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This document contains 164 technical papers on environmental modeling efforts in air quality management, air and water pollutant transport processes, water runoff, water supply, solid waste, environmental management and planning, environmental economics, environmental statistics, ecology, noise, radiation, and health. The Conference was directed toward the technical and administrative communities faced with the need to make environmental decisions and predict future environmental phenomena. The Proceedings are believed to be the most complete summary of environmental modeling efforts currently available.

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FOREWORD

Although many mathematical models have existed for some time in air pollution, water pollution, ecology, and other environmental areas, there previously have been few attempts to bring these models together to create one scientific field unto itself. This conference, the EPA Conference on Environmental Modeling and Simulation, is a first attempt to bring together the many diverse environmental modeling efforts in order to form a unified discipline—*environmental modeling*.

The Conference Proceedings are believed to be the most complete single resource document currently available covering the state-of-the-art of environmental modeling in a variety of environmental fields.

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CONFERENCE BACKGROUND

Elijah L. Poole
Office of Planning and Management
U.S. Environmental Protection Agency

It is my unique pleasure to welcome you to the "EPA Conference on Environmental Modeling and Simulation." This is the first EPA conference where modeling and simulation will be discussed in so many diverse topic areas: air, water, pesticides, solid waste, noise, radiation, health, energy, ecology, planning, management, economics, and others.

The Environmental Protection Agency was established in 1970 to permit coordinated and effective governmental action in order to protect the environment. Two of its roles are to perform research and to transmit research results to the users. In general, mathematical modeling and simulation are widely used for performing research, and this appears to be particularly true for environmental research.

We were overwhelmingly pleased to receive 220 abstracts as a result of our call for papers, and 164 papers are scheduled for presentation at this conference. These papers indicate considerable and extensive environmental modeling efforts in EPA, State and local governments, universities, and private industry. Some papers also were contributed by modelers from Canada. We feel that we are indeed fortunate at this conference to have so many distinguished speakers and attendees - many of whom are well known experts in their fields.

Some major objectives of the Conference are: to perform a state-of-the-art review of predictive modeling and simulation in the environmental decisionmaking process, to share modeling expertise within and across various media, and to better understand computer requirements and other resources needed in the development and use of models.

Considerable efforts are expended in formulating and developing mathematical models, and a large share of computer time is spent running modeling programs. This conference should serve to enhance communication among modelers and users of models, thereby decreasing development and operating costs and also eliminating some redundancies. With the expertise represented here, I feel that many of the Conference objectives will be accomplished.

The Conference has been in the planning stages for more than a year. It was some 18 months ago that Dr. Wayne Ott of the Office of Research and Development and I discussed the feasibility of structuring a conference on environmental modeling and simulation. Prior conversations with many of the Agency modelers and users of models supported the usefulness and desirability of such a conference, and so now the concept has come to fruition.

Many people have been involved working to make the Conference a success. The list is rather long so I will not take the time to try and name everyone. In the back of your program guide you will see an extensive list of primary contributors beginning with Vern Laurie, the Conference Coordinator, and Delores Platt for logistics. And, of course, there are many others whose efforts are appreciated.

In general, the program is organized according to subject matter. The Program Committee felt that some papers were of considerable interest and should be presented, although no topic category may have existed. Because it was decided not to have a miscellaneous session, you will occasionally find a paper in a session where it may not seem to belong. This happens rarely, however.

It is our hope that all attendees find the Conference stimulating and discover new techniques and contacts for future references in developing, operating, and using models.

CONFERENCE GOALS

Albert C. Trakowski
Deputy Assistant Administrator for
Monitoring and Technical Support
U.S. Environmental Protection Agency
Conference Moderator

I believe we have opened a new chapter in the environmental sciences by holding this conference. For the first time we are bringing together, under one roof, all the many varied and diverse environmental topics where mathematicians, statisticians, operations research specialists, systems analysts, engineers, and others with quantitative backgrounds share a common interest.

It is unfortunate, I believe, that modelers working in air pollution seldom have a chance to become fully acquainted with water pollution modeling approaches. Similarly, computer models in solid wastes seldom are brought to the attention of persons developing models for economic studies of air pollution. Models developed for noise applications probably are not widely known among the air or water pollution modeling communities, and models concerned with ecological processes do not often appear in the literature alongside papers on environmental statistics.

There is, however, a commonality of approach among modelers. This commonality should enable them to communicate freely and effectively once they are brought together in a forum such as the present conference. Although mathematics and statistics form the foundation for this commonality, the universality does not end there; there is also a commonality of purpose among the modeling community.

Most models are based on, or make use of, environmental data in some form--particularly monitoring data. Also most modelers, by developing abstractions of reality, attempt to simulate reality. By examining the behavior of their model under a variety of situations and with different inputs, they often make predictions about reality. The "rightness" or "wrongness" of these predictions is, of course, model validation. Models also share many similarities in terms of applications and uses. Some of the more common uses are to (1) project future environmental phenomena and variables; (2) develop more optimal control systems and technology; (3) gain insights into underlying physical, chemical, or biological processes; (4) evaluate the consequences of various environmental management decisions and regulatory strategies; (5) assist in the planning process; (6) aid in the interpretation and analysis of monitoring data intended to depict the state of the environment; (7) estimate the risks of adverse effects of environmental pollution on human health, plants, and animals; (8) assess the economic and social costs arising from environmental pollution.

Our goal in planning this conference was not, however, merely to bring modelers from different environmental media together for them to share thoughts about the nature of models. Rather, our goal was to seek a confrontation between the model users and the model developers. Thus, you will see that the Conference Program contains some very interesting papers discussing the practical experience of environmental managers with models. In several instances, we have included papers from state and local environmental control officials who will tell us the problems and successes they have had with particular kinds of environmental modeling efforts. We hope that the question and answer periods in the technical sessions will stir some lively debate on these matters. Hopefully, by bringing model users and model developers together we can accomplish a better understanding of the potential uses and limitations of models at the same time that the developers receive some constructive feedback from the users.

This brings me to some comments about the role of the Environmental Protection Agency in the modeling areas. EPA's Office of Research and Development serves as the major scientific and technical arm of the Agency, carrying forward a broad and varied research program covering air, water, energy, ecology, and many other facets of the environmental sciences. This research program includes both in-house and contractual work directed toward the development, testing, evaluation, and refinement of models for all environmental media. Within the Office of Research and Development, the Office of Monitoring and Technical Support is the primary organizational entity responsible for transferring the technology produced by the research community into the hands of the user community. We view this conference, which is cooperatively supported by EPA's Office of Planning and Management, as one of the more important means by which the results of scientific research (in this case, environmental modeling approaches) can be effectively transferred to the user community. Thus, we hope the conference will help facilitate a productive dialogue between the developers of models and the environmental managers faced with the need to make decisions using the results of these models.

TOWARD A COMMON LANGUAGE

KEYNOTE ADDRESS

Dr. Andrew W. Breidenbach
Assistant Administrator, Office of
Water and Hazardous Material
U.S. Environmental Protection Agency

As a scientist and a decisionmaker within the Environmental Protection Agency, I am struck by the fact that this conference is long overdue. It is the first conference on modeling and simulation to bring all the various media of the environmental community together. In looking over the schedule for the next two and a half days, I note that at least 15 distinct areas are represented, including air, water, energy, solid waste, ecology, noise, health, and radiation. Five years ago, before EPA existed, this conference would not have been possible, but today it seems quite natural to consider multi-media approaches.

This conference is important to me because scientists and modelers are playing a very active role in decisionmaking today. As our decisions become more complicated, scientists are working more closely with the decisionmaker. By visiting with you, I hope to learn more about modeling. At the same time, I hope I can convey to you some of my thoughts, so we can establish a basis for communication between modelers and decisionmakers.

GETTING DEFINITIONS STRAIGHT

Good communication begins with a common language. I ask you to recall the situation not too many years ago when Congressmen and Administrators shuddered at such terms as "Biochemical Oxygen Demand," "Total Suspended Particulates," "polychlorinated biphenyls," and "oxides of nitrogen." These words probably sounded more like Greek than English. But let us look at how far we have come in just a few years. Most Congressmen know that "BOD" has something to do with sewage treatment plants. Even such terms as "ozone layer" and "catalytic converter" are household terms. I think we have come a long way toward bringing the language of the scientist within the province of the decisionmaker.

But the language of models is another story. Take the simple word "model." How often has someone come into my office and mentioned that he has a model, and I wait expectantly for her to come into the room. Or for a large display case to be carried in with a miniature replica of a waste treatment plant. These are not unusual reactions when hearing the word model. We have become accustomed from childhood to such concepts as "model T," "toy models," or "you should model yourself after that person." All of these examples imply that a model is a physical representation.

The dictionary's definition seems to focus on this physical aspect. Webster defines a model as "a standard for imitation or comparison; a pattern. A representation, generally in miniature, to show the construction or serve as a copy of something." Actually this is not a quote from Webster, but from the Random House Dictionary, which I thought would be more appropriate for this conference.

Nowhere does the dictionary, or for that matter, the decisionmaker's general experience, really depict the idea of a mathematical model. Yet from what I can gather, almost all of the models you will hear about this week are mathematical models of one sort or another.

Even if the decisionmaker understands the concept of mathematical model, he is likely to be confused and overwhelmed by the variety and complexity of available models. This confusion could lead to a serious breakdown in communication. For instance, the decisionmaker may have in mind a simple, deterministic model, but the scientist may actually be using a statistical model, or a stochastic model, or a simulation, or an analog computer model.

It is important to get our definitions straight and agree on a common language. Since the language of modeling is unknown to the public and to many managers, the subject seems to cause some fear, or at least a feeling of distrust. It is only human nature to be a little afraid of something new or something you do not understand.

A COMMON LANGUAGE

A simplified and clarified language of modeling will go a long way in advancing the cause of modeling. Managers and the public will better appreciate modeling, and as appreciation and understanding of models grow, so will the use of models.

A careful and consistent language of modeling can also help communication between modelers. As you listen over the next few days to the many talks on models, think of how many different ways you hear the word "model" used. In the titles of the papers to be presented, the words "modeling" or "model" occur 107 times. One would expect that for such a common word, each of us would be well acquainted with its meaning. Yet, when you listen to papers being presented, ask youself whether you really know what the authors mean by the word "model." Better yet, consider whether you think your neighbors on either side of you have the same concept of "model" that you have, and that the authors have. I suspect there may be a good deal of fuzziness in the definitions commonly used.

Another major reason for my concern about definitions is that we are frequently being sued over our decisions, both by industry and by environmentalists. Courts must listen to both plaintiff and defendant discuss modeling. Since neither the plaintiffs, the defendants, nor the courts can define their terms exactly, I can almost guarantee that opposing sides will disagree on what they mean by "model."

Thus, development of a consistent and understandable modeling language is becoming extremely important to the manager, the scientist, and the public.

We will not, however, be able to develop a common language overnight, and even if we attack the problem over the next two and a half days, we may not get very far. But there are some reasonable first steps we can take. As the keynoter for this conference, let me propose some questions from my perspective as a decisionmaker to help define what I mean by a common language. As you hear about models in your area of concern, whether it be water quality, ecology, or economics, keep in mind what decisionmakers like me need to know.

CURIOSITY OR DECISION TOOL?

One question might be, "Is this model a mathematical curiosity or is it a tool for making decisions?" I know that we have advanced well beyond the mathematical curiosity stage but I am not sure whether we have arrived at the decisionmaking end of the spectrum as yet.

To help find out where we stand in the evolution of models, let me describe the results of my own model which I commissioned solely for this conference. The model is called A Statistical System to Evaluate Symposium Success, also known as ASSESS. My staff assures me that it is a state-of-the-art model, with nothing but the best data inputs, and the most rigorous of validation techniques.

We performed a keyword analysis on the titles of all 164 papers to be presented here this week. Then we classified the papers into three categories: Policy-Oriented, State-of-the-Art Review, and Technical.

We called a paper Policy-Oriented if the title of the paper had the slightest hint of policy orientation, such as by using the words "planning," or "management," or "policy." Of course I hoped that 95 percent would be Policy-Oriented papers. In reality, we found that only 17 percent of the papers fell in this category. So I doubt that we have reached the stage of model evolution where all models are being directed at policy questions.

The next category is State-of-the-Art Review. These papers perform a valuable service to modelers and decisionmakers by comparing and analyzing models. Twelve percent of the papers fell in this category. I hope we will see more of this kind of paper in the future.

The third category is Technical papers. If the title of a paper did not mention policy, and did not appear to be a review, we called it a technical paper. By now you will not be surprised to learn that the majority of papers—71 percent—appear to be Technical papers. These figures suggest we may have too many models which are still in the mathematical curiosity phase. I hope not.

I do not wish to imply that all technical papers are irrelevant to the decisionmaker. I know that many are very relevant. My point is that the modeler must become more sensitive to decisionmakers' needs, and must know how they intend to use the model.

So much for the ASSESS model. I know the conference will be a success in spite of it.

ASSUMPTIONS

Another question I ask as a decisionmaker concerns the model's assumptions. Assumptions do for a model what gasoline does for an automobile—they make it run, and they determine how far it can go. The person who developed the model probably knows precisely what assumptions are important. It is the user—the decisionmaker—who will feel the effects of these assumptions.

The decisionmaker must be told if there are assumptions which are simply not true and which completely invalidate the model. Unfortunately, modelers can become so involved in making the model work that they forget to distinguish between things that are true and things that are convenient simplifying assumptions. The user must know, for instance, if a model is only for lakes, or if it assumes complete mixing, or if it is valid only for summer months. Stating the assumptions is a key part of the common language of modeling.

SENSITIVITY

I also like to ask about the sensitivity of the model to input variables. The decisionmaker must be told which variables are critical to the results, and which variables do not impact the results. One of the most useful outputs of models is this ability to distinguish between what is important, and what is unimportant. So sensitivity analysis should also be a part of the language of modeling.

VALIDATION

One of my favorite questions is, "Has this model been validated?" Sometimes it may be impossible to validate a model completely. For instance, a global economic growth model may be difficult to validate. But to use a model in making a decision, I must have some proof that the model works, or at least have something which convinces me I can rely on it.

The only sure way to validate a model is to test it using new data—that is, test it using data which were not used to develop the model. In the water program, we have often found models which people claimed were valid, but were really just tested with the same data used to develop and calibrate the model. This is like using a pocket calculator to verify that x+y = y+x, for all the possible values of x and y. When you test a model with new data, you are also helping to determine how robust the model is—that is, how applicable the model is under varying situations.

Validation is not something to be afraid of. Validation techniques can improve your models in the long run, even if they show that your present model is incorrect for the task at hand. And I guarantee that decisionmakers will use your model more willingly if you have solid evidence to validate it.

DATA INPUTS

One final question I often ask is," What data did you use? Did you collect the data yourself, or did someone collect it for you? Are the data valid today, or are they obsolete? What variables were measured?" I can assure you these are not empty questions. We have found treatment models which use temperatures as a key independent variable, but which were based on input data collected at a constant temperature. We have also found a water quality model for a particular river, where all the so-called ambient monitoring data were collected just downstream from industrial outfalls. A good corollary to the "garbage in-garbage out" rule is that a model is only as good as its data.

The quality of data used is probably one of the restraining forces for the modeling community today. The high costs of collecting data are enough to make some managers shudder at the word "model." Yet, it is the modeler's responsibility to insist on good data, even if it means higher cost. If good data are not available, the modeler should point out how this limits the validity of the results.

DECISIONMAKING AND RISK

Why ask these questions? Why worry about who uses the model? About assumptions and sensitivity? About validation? About data? The reason is that as a decisionmaker, I cannot afford to use a model which is wrong. For once a manager uses a model which turns out to be wrong, he will probably never want to use a model again.

Consider the county executive or State governor who makes a decision based on an urban transportation model for air pollution, or a stream loading model for water pollution. What will be his reaction after the new parking plan is implemented, and the air is still dirty? Or after the new treatment plant is built, and pollution does not improve? Not only will the modeler's reputation suffer, but the momentum of the entire environmental movement could suffer seriously.

The public manager wants to minimize his risk of making wrong decisions. And that, in a sense, is one of the primary justifications for developing models in the first place. It is your job and responsibility as modelers to reduce the manager's risk.

THE BIG PROBLEMS

In the water program, decisions are made routinely using models, or so I am told. Models are used to help determine effluent guidelines, determine water quality standards, and evaluate the impact of effluent reductions on water. We could not set standards for "best available technology," for instance, without the use of models, since in many cases the technology does not exist in widespread use. Water quality criteria could not be established for many materials without using mathematical models. Mathematical models are well known in toxicology and help the scientist determine the relationships between doses for animals, aquatic life, and human beings. Models help us determine what amount of pollutant in the water will yield a cummulative toxic dose in aquatic organisms. Effluent loading models can help determine the impact of our multi-billion dollar cleanup programs.

It was my intention when preparing this paper to give examples of modeling success stories. Yet with all of these models in my program, we could not find one which was universally acclaimed for solving what we call a "Big Problem." A Big Problem is a problem that makes the press, that causes Congress to come screaming and yelling at our doors. To be sure, we have many examples where a model was used to help make a local decision. Yet many of these models were unreliable or controversial and, in the final analysis, decisions were sometimes made on the basis of common sense as much as they were on the model.

I interpret this to mean that modeling has been in an embryonic state. I hope that you, the modelers, through this conference and your interaction, will help modeling come of age for the Big Problem.

I believe that models have a lot to offer the manager. That is why I would like to see both managers and scientists start working with more urgency on the problem of developing a common language. If a dialog is initiated, the modeler will begin to get a better idea of what the decisionmaker faces. Models to solve the Big Problems could begin to be developed. And the decisionmaker will have better information to confirm or deny his common-sense beliefs. As environmental problems become more complex, the decisionmaker depends more and more on technical knowledge. Models can help focus this knowledge, and help us solve some of these problems.

CONCLUSION

The organizers of this conference have done an excellent job of bringing together many diverse entities. The program is so diverse, and the time is so short, that you will only be able to hear a small portion of the papers to be presented, even if you spend all of your time at conference sessions, and not at the bar downstairs or watching the World Champion Cincinnati Reds. All of these papers, and the stimulating dialog with your counterparts should ensure that we meet the major objectives of this conference. These objectives are, and I quote:

> "To perform a state-of-the-art review of predictive modeling and simulation in the environmental decisionmaking process; to share modeling expertise within and across various media; and to examine the adequacy of computer and other resources in the development and use of models."

As we embark on this conference, I give you the task of creating a common language that both modelers and decisionmakers can readily understand. This language will also help convey our decisions to the general public. I also give you the task of creating a consistent methodology for verifying models and describing their capabilities, so that managers will have a standard with which they can measure the usefulness and accuracy of models. Armed with these, the modeler will be able to convince more and more managers to use models in environmental decisions.

A RESOURCE AND ENVIRONMENTAL MANAGEMENT EXCHANGE

LUNCHEON ADDRESS

Dr. Ira L. Whitman
Environmental Engineering and Management
Columbus, Ohio

The conference coordinators advise me that this meeting is dedicated to the *users* of modeling efforts, to individuals in government and industry whose management and planning efforts will determine the future course of resource and environmental management.

What I have to say should be of interest to anyone concerned about the future of environmental management—and should particularly concern you modelers and analysts who care about the results of your efforts and the impact that you have on the environment. I will plead my case for an awakening, a *humanization* of technical persons working in the environmental professions. Also, I will offer a plan to create leadership in the environmental field, leadership capable of dealing with real-world problems founded upon a solid scientific and technical base.

I can personally recall that day, almost 15 years ago, when I first interviewed with my graduate advisor to be, and learned that in exchange for tuition and stipend I would be transforming unit operations of sanitary engineering into analog computer simulations. However, it wasn't until several months later that I learned what an analog computer was. It took even longer to recognize the fantastic potential for discovery that existed with the use of models, simulation and with computers. My efforts were modest by comparison with yours, yet they were sufficient to crank out that all-important Master's thesis, and send me off to the cruel hard world where there is no equation for reality, and no model that tells us when and how to make the right decisions.

I decided to leave the models and computers to others, and attempted to build upon their expertise in environmental modeling to bring about more rational environmental policies and better managed environmental programs. In 1971, in Ohio, we introduced the concept of effluent charges to the Citizen's Task Force on Environmental Protection, a concept that was endorsed by a coalition of environmentally oriented citizens and businessmen above the protests of the industrial community. In 1972, we quietly commissioned a study of an industrial cost sharing approach based on computer modeling of major air pollution sources in one of our industrial cities. Also in that year, we hired some of the State's first environmental modelers, who have distinguished themselves by presenting no less than three papers here at this conference. Yet, in 1974, a major enforcement case we were pursuing was hopelessly lost, due considerably to our failure to validate critical air quality monitoring data.

The lesson learned from these experiences is this: There is an undeniable linkage between the major elements of a national program of resource and environmental management. I see four such elements, each being a link in the process of achieving our national environmental goals. These elements are:

1. Scientific monitoring and understanding of the components of the environment.

2. Integration and analysis of these components into understanding of environmental systems, through modeling and other systematic tools.

3. Formulation of environmental policies, and administrative and legislative actions in order to *manage* our environmental systems.

4. Implementation of environmental programs including design and construction of facilities.

Scientific monitoring and research allows us to identify and describe the components of our environment. We must know what these are before such systems can be modeled and analyzed. Much of *your* work has been restricted by limitations in our basic data and our knowledge of natural processes. Ecological modeling, for example, is only as good as our knowledge of the basic ecological processes themselves, many of which we understand in only a primitive fashion. Millions of dollars now go into basic environmental data collection—from ships, balloons, space satellites, and from complex and very simple monitoring equipment here on earth. The outputs from this first phase of environmental inquiry are the raw inputs needed by you, the modelers, mathematicians, and analysts.

Environmental modeling and simulation are integrating processes, by which *relationships* are tested and explored. Through modeling, we can integrate the biological and chemical factors that describe a polluted waterway with the cost and benefit factors that describe the results of improving that waterway, thus gaining economic insights into the impacts of physical phenomenon. The horizons of your models have become elasticized by new generations of computers and new generations of modelers who have ingeniously learned how to represent a physical world by an electronic world.

But what of the results of your modeling efforts? Where do they lead and where have they gone? How many "optimal" solutions have become "acceptable" solutions? How many "least cost" alternatives have become "most used" alternatives? Where have your models taken us?

You have led us, I believe, to the doorstep of that next element in our environmental programs, the formulation of policies, and administrative and legislative actions. But have you taken us across the threshold? Rarely! It is this realm of policy and administration that concerns me the most, for this is the *real* world—the world of people and their problems; it is the place where push comes to shove—not just in our models, but in our city halls and board rooms and anywhere that real power is being bartered and brokered.

Ah--but you say that it is your job to provide the data and the alternatives, and that it is the decisionmakers who must make the choices. But who are the decisionmakers—and why is it they who are playing chess with our resources and our lives while you, who have the tools of understanding at your command, are playing second fiddle?

So the question I ask is this—how do we integrate the rationality which you, as modelers and analysts, can provide into the real world of the political pro and the board room Machiavelli?

Can we bring the decisionmaker to you and convince him of your wisdom? Can we wrap you up in a nice neat shiny package and bring you to his world? Will he listen? Will he understand you?

NO!!

How do your models, and what they have to offer, get across that doorstep into the real world where the action is? My friends, you take them across. Hand-carry them—special delivery. And how do you guarantee that they are actually delivered, and that they find their way into the thought processes that lead to action? You must be there on the other side waiting to receive them, and willing to put them to use.

Become the decisionmakers! Not through your models, but through yourselves—your talents, your words, your actions, your interests. Prepare yourselves to put behind you the world of computers and to professionally inhabit the world of people. You will find a vacuum there waiting for your leadership, and the vacuum created in your wake will soon be filled by new generations of modelers waiting and following behind you.

If you expect the leaders, the decisionmakers, to understand and embody the work which you are performing, then you must prepare to provide the leadership. I am suggesting that you, the mathematicians, modelers, and engineers, become humanized to the point where your concerns are with the use, the impacts, and the practicality of your plans and the results of your modeling efforts. In short, no environmental policies and programs in this country, nor any public policy, can grow and evolve towards the achievement of their goals unless the persons best trained and equipped to understand and implement those policies grow with it. Grow!

I believe that many of you must set out to reorient yourselves and grow, in two directions which will enable you to become a part of the decisionmaking process. Grow in the direction of your personal actions and behavior, and grow in the direction of your professional interests and career.

Grow by communicating! How often have you heard the word communicate thrown up to you—at professional meetings, in your office, and anywhere where people are concerned about the results of your labors?

Communicate! But do you really? Can you describe your work and its applications to your wives? How many of you are understood by them well enough so that they would be able to describe to others what you do?

What about your kids? Do they understand what you do? Have you ever spoken to their classes in school? If you have, did you get your point across well enough so that your kids were glad you came? Do you think you could explain to a 6th grade class what you do, and why it will help fight pollution in some way? What about an 8th grade class? 10th grade? 12th grade? Could you, in fact, successfully speak before a class of college sophomores? Could you do it without writing equations on the board?

Several years ago, my kids, very young at the time, were confused by the fact that certain people called me Dr. Whitman, yet whenever they were ill their mother would have to take them to visit the pediatrician (and usually complain about the cost as well). What kind of a doctor was I that I couldn't treat sick kids? After much attempted explanation, it all crystalized when I explained that I was a "doctor of sick rivers," and not a doctor of sick children. Children's perceptions of pollution are very vivid, and very real. Cleanliness is usually the first concept driven home to kids by their parents—and violation of public cleanliness, pollution, is not an abstraction to them by any means. It is what you and I are doing to clean up the pollution that becomes the abstraction. In their simplified world, mother always has an immediate solution for the pollution problems which concern them. Yet we, whose business and profession it is to clean up on a larger scale, seldom produce results, or even take actions which the kids can comprehend. Well, if they in their enthusiasm cannot know what we do, what makes you think that the public at large will?

If your kids, or the ones down the block, can't understand what you're doing, what about your parents? Have you ever tried to explain your professional activities to your parents and to members of their generation? They want to know that the country which they fought for 35 years ago, and which they helped rebuild after a disastrous depression, is being left in good shape for their grandchildren. They don't care too much about our generation—if things are a mess they figure it's our own fault. But they surely care about our children! What have you done lately to assure our senior citizens that you are helping to produce a healthful and safe environment for future generations? Do they understand you? Do you talk to them at all?

Communication is just the beginning! How about involvement in community problems—environmental or otherwise? I know that many of us "working stiffs" in this field are getting involved, be we modelers, or lawyers, or technicians. Much of the acceptance of public involvement in environmental policies and programs has come about because some of us have been involved, and are beginning to understand what citizen action really means.

How about involvement in the political process? How many of you (federal employees excluded!) have ever seriously participated in the election of a candidate? Have you passed petitions from door to door and tried to explain why your man was better than the other guy? Have you ever cornered and interrogated a local candidate to find out what he really stood for? Have you sat in on legislative hearings—only to wonder what was really decided behind closed doors before the hearing ever began?

Why am I dwelling upon the theme of communication and involvement? Because they are part of personal growth. Unless you share experiences with other people, experience their interests, their feelings, their views, their preferences, their philosophy of government, it will be impossible for you as an economist or mathematician or scientist to take your efforts into the real world where it all happens. I'm talking about the world beyond the doorstep where so many of our academic exercises come to rest.

But self-help is not always enough! There are those of you out there, and colleagues of yours around the country, who would like nothing better than to have the opportunity to take your talents to the board room, and to city hall, and to apply yourselves not just to the description and modeling of the environment, but to participate in the decisions and the actions which lead to the management and protection of the environment.

To enable this professional growth to happen, I am proposing a Resource and Environmental Management Exchange, for the purpose of developing responsible, well rounded, experienced men and women capable of exercising leadership in the private and public sectors in dealing with environmental and resource issues. This is the first public announcement of this concept which has been brewing for months, and which will be put before leading governmental and private organizations concerned with our ability to manage and protect our natural and environmental resources. The objective of the Exchange is not to take technocrats and let them manage our resources, but rather to build upon persons who have strong technical experience in the environmental field and help them become fully rounded, sensitive, alert participants in the management and policy-making processes.

The Resource and Environmental Management Exchange would, with the commitment of the individuals and organizations involved, establish over a five-year span the capability we need to manage our environment and our resources intelligently and democratically. Just what commitment do we need?

At the start, I would envision an Exchange which has the backing of some 75 to 140 organizations, involving 200 individuals. These individuals would be presently employed, as many of you are, by large and small corporations, states, universities, units of our federal government, think tank and research centers, local and regional agencies, and professional societies. Each organization participating would be committed to the following:

1. Selecting and sponsoring one or more of its staff for involvement in the Exchange over a five-year period.

2. Underwriting part of the cost of its employees' participation in the Exchange, including seminar and involvement programs held regularly over the five-year period.

3. A willingness to exchange personnel with other participating organizations for periods of 6 to 18 months.

4. A commitment to build management opportunities for Exchange graduates.

I estimate the cost of this program to be from $3,000 to $4,000 per year per person, which accounts for all costs above the normal salary and other costs of employment for Exchange participants over a five-year period. For a complete Exchange group of 200 individuals, this results in a total cost of $4 million over the five-year period.

But what are the potential benefits by which this cost can be measured? What is the price of leadership? Corporations now spend thousands of dollars in training and upgrading their management team members, and in relocating them throughout their organizations. The cost of hiring new management talent into their organizations is even higher. The current value of environmental programs—public and private, is in the billions of dollars a year, and still growing!

We have spent millions on environmental monitoring, and data collection, and more millions on models and computer analyses to try to generate some sense of these data. Yet, by and large, we deliver the results of our efforts to persons in organizations, private and public, untrained in management and unaware of the benefits which national resource management can really produce. And, even more alarming, policy and management actions lead to programs costing billions of dollars in the construction of waste treatment facilities, in the prevention of adverse environmental impacts, and in the cancellation of facilities that might otherwise be built. As various need surveys show, the total cost of meeting our environmental goals lies somewhere between our annual federal budget and our gross national product, both of which are very large amounts, to say the least. Can you imagine what the value of improved management and alert leadership in these programs will be? That is why this program is being proposed—to bring us the professional growth and leadership that is needed.

Through modeling and simulation we have been able to integrate many factors within our environmental and economic systems. We can make trade-offs leading toward solutions that offer us the most for our money. Through your efforts we can study the response of air sheds to new development, the change in river quality as we progress with our pollution cleanup efforts, and we can electronically track garbage trucks as they find their way around a large city over assorted hypothetical routes.

But now we must do more than model the environment and simulate our management systems. We must harness the talent which has been used to develop these magnificent tools and give it the opportunity to grow and to prepare for the responsibilities of leadership. We must steer ourselves toward people, for it is they, and not our machines, who will determine whether, and to what degree, our environmental goals will be met. And, in building this leadership, we should consider the institution of efforts to expose our talent to new situations, new experiences, new pressures, and new responsibilities. In short, we need to consider something like a Resource and Management Exchange, which will allow us to build upon our scientific and technical skills and develop this leadership for the future. With it, we all grow!

I hope you agree! Please let me have your ideas, and your response to these ideas.

FUTURE ENVIRONMENTAL QUALITY MANAGEMENT
USING MODELS

David W. Duttweiler
Director
US Environmental Protection Agency
Environmental Research Laboratory
Athens, Georgia

Walter M. Sanders, III
Acting Associate Director for
Water Quality Research
US Environmental Protection Agency
Environmental Research Laboratory
Athens, Georgia

Introduction

The purpose of this paper is threefold: 1) to show environmental pollution control officials and managers the potential of models for enhancing the efficiency and effectiveness of their efforts, 2) to suggest to modelers that their products can be more useful in environmental protection, and 3) to outline a future mode of action for environmental protection that could be superior, in its accomplishments and costs, to the present approach.

The concept of the environment as a system will be outlined and "pollution control" compared with "environmental quality management." Steps to realize environmental quality management through use of models will be described and the potential benefits of instituting environmental quality management will be discussed.

Environment

A useful concept of the environment is a system composed of sources of materials linked by transport and reaction processes to biological receptors or sinks where the materials are sequestered from further significant environmental activity. The materials are usually residuals (wastes) of human activity, occasionally materials intentionally injected into the environment like pesticides, and often the products of geochemical processes. They become pollutants when, for reasons such as health, ecology, economics, or aesthetics, they are undesirable constituents of one or more abiotic environmental components (media), such as air, water, or land. The atmosphere, for example, transports a pollutant from its source to receptors or to sinks, which may be organisms, another environmental component, or man-made objects. During transport the pollutant may participate in chemical or physical reactions that may transform it into other materials that may also be pollutants or that may give further rise to pollutants. Pollution occurs when adverse effects attributable directly or indirectly to the pollutants are discerned in receptors, or when the "quality" of the medium is degraded to a level that impairs its utility. Fishkills and saline agricultural irrigation water, respectively, are two obvious examples.

Pollution Control

The contemporary approach to eliminating or preventing the undesirable effects of pollutants focuses, logically, on their sources, but virtually ignores the rest of the environmental system or treats it piecemeal. Pollution control is based on technological or managerial modification of pollutant sources that either emit greater amounts of pollutants than society deems reasonable for such sources, or that cause pollutants to appear in air or water in amounts that society finds unacceptable. Pollution control is generally confined to sources that affect a single medium; rarely are effects in other media considered.

Environmental System Management

A superior approach to solving society's environmental pollution problems, employing a holistic view of both the environment and society, would allow the environment to be managed to achieve the objectives society chooses. Advocated by both environmental technologists and social scientists (for example, McGauhey, 1968; Freeman, et al., 1973), a system management approach could devise means of attaining society's objectives most effectively and efficiently. Management of the environmental system, rather than its individual components, should prevent the unanticipated adverse effects that result when the solution of one environmental problem creates several more serious ones.

The systems approach forces recognition of the interconnectedness of environment and society, and provides a means of evaluating the impact of projected social changes on the environment, and of environmental changes on society. Unfortunately, social systems are understood as poorly as environmental systems.

Environmental Management Functions

We recognize six major steps in the systems approach to environmental management. First, the community's objectives must be clearly identified, and criteria must be developed to judge their satisfactory attainment.

Second, the system to be managed must be defined. Its components must be identified at a useful level of resolution. The boundaries of the system must be delineated and all significant inputs and outputs at the boundaries must be quantified. The processes linking the components must be identified and quantified.

Third, the functional relationships between the objectives and the environmental (and social) system must be adequately quantified.

Fourth, strategies must be formulated that permit a sufficient variety of alternative decisions to be examined for their environmental and social consequences and for their ability to achieve the objectives.

Fifth, an effective means of implementing the decisions must be established.

Finally, a means of measuring the results of implementing the decisions must be provided, and data on environmental and social impact must be made available for use in any of the preceding steps.

Each of the above steps, so easily stated, represents technical, as well as managerial and political, challenges that are not likely to be met satisfactorily without considerable rational simplification. For example, one could not possibly define every input and output of a watershed, since measuring every component of mass transport across the shed boundaries in the real world would be an insurmountable task. However, the dominant processes of the environmental system can be measured sufficiently well to account for much of the system's behavior. Although such incomplete information about the system will prevent full explanation of many of its phenomena, nevertheless it can usually allow rational, system-wide decisions. Simultaneously, areas of ignorance that must be addressed to improve system management will be identified.

Even the simplest of environmental processes is affected by a complex of interacting environmental factors whose net effect is difficult to analyze mentally. Systematic study of these factors and their relations to the process can yield insight that can be experienced by the knowledgeable environmental scientist as a mental picture of the process. Even better, these insights can be expressed as a quantitative mathematical model. Models of individual processes combined into larger models of the environmental system can be studied more economically and more comprehensively than can the real environment. Outputs of model studies can be analyzed for system response to various input strategies and for insights that would be impossible to gain from study of the prototype.

Modeling

Systems science offers some concepts (see for example, McFarlane, 1964) that help understand the potential and limitations of environmental models. An environmental system is a real-world physical system which can be studied only through a measuring system. The output of the measuring system is a set of observations that is used to construct a mathematical model of the physical system. Observations of the physical system can be compared to the model's description, giving a set of errors that guide refinement of the model. This iterative process continues until the errors become acceptably small. The model is then accepted as adequate to represent or simulate the prototype physical system for the intended purpose.

Some models can be formulated in a way that allows them to be used analytically for detecting interesting features of the system and its behavior. Especially for management purposes, they can find optima, that is, find a set of conditions that will cause an objective function (an objective stated mathematically as a function of one or more system variables) to take on a desired maximum or minimum. For example, the minimum value of the cost function for a set of pollution control procedures can be found through mathematical manipulation. Some models can only be formulated in a way that requires the objective function to be searched for the optima. Even with this restriction, however, searches using models are usually much more efficient for finding the optima than are searches in the real world.

Models must not be confused with their real-world prototypes, and conclusions drawn from them must be applied with caution. A model built with one objective in mind will likely be inappropriate to simulate the system for a different objective. Models built without clearly defined objectives may have no practical use in solving environmental problems. Models that are not periodically compared with their prototypes can become treacherously inaccurate if the prototypes or constraints change without detection.

Mathematical models are perhaps the only feasible means of accomplishing the six major steps outlined for system management. The setting of social objectives is an especially complicated process in a democratic society. Models of this process and the interactions between society's various objectives can suggest efficient means of optimizing its results. Objectives set by any process, however, may be unanimously desirable, but not feasible. Models that relate objectives to the systems to be managed can give insight into their feasibility that might otherwise await actual failure of attainment. An imprecise or non-feasible objective can often be recognized and an equivalent feasible objective substituted as a result of such modeling.

The quantitative descriptive power of models is essential to define a system to be managed, and to focus attention on its significant features. For a given objective, these features can be described quantitatively so that the variables having the greatest relevance to the objectives can be modeled.

Functional relationships between objectives and the system to be managed obviously can be quantified only through mathematical representations. These functions, known with sufficient resolution and precision, are crucial to the rational application of system management.

Development of alternative management strategies for environmental systems can use the powerful techniques of operations research, mostly based on models, that have been applied so successfully in most other modern industrial and commercial activities. (See, for example, Churchman, et al., 1957.)

If the means of implementing decisions is considered separately, models can be used to design efficient decision-implementing systems and guide their operation. Again, operations research and modern management science offer powerful techniques.

Finally, the design of systems to monitor the results of environmental management decisions should be based on the models used to reach the decisions. Models of the monitoring system itself are useful for optimizing its operation.

The six steps involve a variety of disciplines that traditionally are not accustomed to the team effort that is needed to make system management effective. Semantic and philosophical differences can find a common ground in models and their symbolism.

Environmental System Models

Construction of predictive environmental models is a complex scientific challenge. Recent successes have been confined mainly to models for managing specific materials or controlling the quality of a single medium (see, for example, Loucks, 1972; Thomann, 1972; Deininger, 1973; Hill et al., 1976; Lassiter, 1975; Bloomfield et al., 1973). Environmental modelers are adopting a modular approach that permits any number of subsystem models to be assembled into larger, more comprehensive environmental system models. Such models will never be able to predict reliably every variable and parameter that might be of interest, but they should provide sufficient basic information to meet the environmental manager's needs. Models that offer insight into ecosystem functions that impact environmental quality (Chen et al., 1975), and in the behavior of pollutants in ecosystems (Gillett, 1974; Sanders, 1975) are available in various stages of utility. Models that describe an operationally significant water quality parameter, dissolved oxygen, have been available in useful form for fifty years (Streeter and Phelps, 1925) and are in general use for making water pollution control decisions. Models of the concentration and distribution of atmospheric pollutants are being used for planning and operating air pollution control programs (Singpurwalla, 1974).

Social System Models

Modeling society is as great a scientific challenge as is modeling the environment. The simpler social subsystems, e.g. community activities for solid waste disposal (Liebman, 1974), have been successfully modeled. The social subsystem that has received the greatest attention of modelers is, of course, the US economic system, which continues to challenge econometricians. Models are available for such social functions as community health services (Palmer, 1974), law enforcement (Gass, 1974), educational systems (Weiss, 1974).

Management Models

Logical decision making has benefited greatly from the quantitative analytical techniques developed by operations research. Both processes and organizations for decision making have been modeled for a variety of purposes and in numerous settings. A large body of knowledge on decision making under uncertainty (see, for example, Raiffa, 1968) is available for application by social institutions responsible for managing environmental quality. Regional models that can help identify decisions which minimize the cost of "managing" residuals are available (see, for example, Kneese, et al., 1970; Spofford, 1973).

Implementation

The development and application of realistic environmental management models have been hindered by the difficulty in defining or isolating specific systems to be managed and by the discontinuity of the social institutions having the responsibility for planning and implementing management strategies. Logical geographic subdivisions for one medium seldom coincide with those for another medium; none of the subdivisions match the various state and local governmental boundaries. EPA has had difficulty in focusing on true intermedia programs since its authority and funding are provided by eight separate laws which are either media, material, or source specific.

The future of environmental system management looks much brighter, however, with the creation of the 150 "Designated Area" planning agencies, established under the authority of Section 208, Public Law 92-500, for water quality planning and management. More recently, they have been given increased responsibility for planning air, solid waste, thermal, and noise pollution control strategies (Mellencamp, 1976). The designation of these subregional or sub-basin management areas has greatly increased the degree of resolution that can be achieved compared to the regional or national scale. Given clearly stated objectives and the proper criteria and tools, these planning institutions can devise true multimedia environmental management alternatives that will permit local officials to explore and strike optimum strategies for achieving both environmental protection and other social benefits simultaneously. Using well developed systems models, such agencies can quickly explore many alternative decisions that could not only reduce the cost of managing the environment for social good but also achieve a level of environmental quality not otherwise attainable.

Based on such model strategies and continual feedback from the local area, these agencies could influence the allocation of costs so that they would be shared equitably and could evaluate progress towards goals and provide course-correcting stimuli. We believe that these same benefits can also be attained on a wider scale when the 208 program shifts from the designated area to the state-wide emphasis as stipulated in the law.

In order to achieve these desired environmental and social benefits, the scientific community must greatly increase its efforts to move systems modeling concepts from the realm of scientific research to practical applications. Social and governmental institutions are developing, but well evaluated comprehensive modeling tools, especially those linking environmental and socio-economic systems, are currently not available for their use.

One obstacle has been the system approach's huge appetite for data. Obviously the effectiveness of system management depends on sufficient pertinent data to construct, test, and use the models needed for each step. The formidable complexity of social and environmental systems might suggest that enough data of the right kind is so costly as to be unattainable. We do not believe that data now available, or data that could feasibly be obtained, is insufficient to meet the present needs of models if a relatively gross level of resolution is accepted. Environmental management decisions based on meager comprehension of the entire system will be, we believe, superior to decisions based on near-perfect understanding of one system component and ignorance of the others. Acceptance, initially, of a grosser level of resolution will facilitate the application and subsequent development of system management techniques. The allocation of society's resources to environmental system management can then grow, if necessary, toward an optimum for achieving the stated objectives.

Obviously, we believe that the systems approach to environmental quality management is a desirable option for improving American social action in environmental protection and one that deserves more consideration, development, application and evaluation.

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A SYSTEMATIC APPROACH TO REGIONAL WATER QUALITY PLANNING

G. Paul Grimsrud and E. John Finnemore
Systems Control, Inc.
Palo Alto, California

Summary

This paper describes the methodologies developed for regional water quality management planning on the Snohomish and Stillaguamish River Basins in the State of Washington. These methodologies were specially designed to be responsive to future changes in state and federal legislation, land use, economics, population, employment, geographical and political boundaries, technological development, and changes in the natural or man-made conditions of the water bodies. Computer models were developed and utilized to project future sewage and runoff flows, determine the assimilative character of water bodies, plan and cost various alternative wastewater management plans and provide other information on the cost-effectiveness of alternatives necessary for the completion of the Water Quality Management Plans. The modeling and programming elements are the principal factors allowing the development of a dynamic and easily updated Water Quality Plan.

The approach is applied to river basin planning on the Snohomish and Stillaguamish Basins, demonstrating its application and results. The methodologies are presently used by planners in Snohomish County for ongoing water quality planning.

Introduction

Planners and managers responsible for the performance of water quality planning programs must usually deal with the complex engineering, economic, financial, legal, institutional and environmental aspects of water quality. They must face the need to develop or acquire a systematic approach to planning which can take all of these factors into account. This paper presents a water quality planning methodology which includes most up-to-date technology for computer-based modeling, yet great flexibility for practical use. The methodology is designed for the selection of most cost-effective wastewater management schemes in a region, and the time-phased design of such schemes over many years in the future. The methodology was developed under contract with EPA, and used on the Snohomish and Stillaguamish River Basins in Washington State.

Planning Procedure

The planning steps followed in the quest for a cost-effective water quality management plan[1] for river basins include the selection of alternative configurations for treatment facilities, carrying out assimilation analyses for receiving waters, costing the alternative configurations, and making cost-effectiveness comparisons. The methodologies employed in these steps are a compromise of computer-oriented quantitative procedures and planner-oriented qualitative activities.

Figure 1 summarizes and clarifies the interdependencies of the tasks in this planning methodology and illustrates the flow of events - prerequisites, bottlenecks, critical paths, progressions. The starting-point data or inputs to the planning process are listed in Column 1 (left hand side). The flow paths to the right from these starting points show the impacts of the input data on subsequent tasks.

Throughout the formulation of planning methodologies, weaknesses in present available information were found. It was evident that certain plan inputs, such as the water quality standards, were likely to change in the near future, thus causing a need for plan updating. These problems were given foremost consideration in the development of plan methodologies. Future updates to the inputs (data or assumptions) should only be made directly to items in Column 1 of Figure 1. Thus, whenever any input to the plan development process is significantly changed at some future date, the flow paths of Figure 1 will identify the downstream tasks in need of review and possible re-execution.

Of prime concern in the development of an effective water quality plan are the concentrations of pollutants in the receiving waters of the basins. Since the natural movements of these waters, and hence their transportive and diluting effects, are ever-changing and variable, some specific flow regime must be selected for planning purposes to make possible the comparison of alternatives.

Flow Regimes

A specific flow regime, for analysis purposes, is required to provide the basis for the computation of receiving water qualities. Although the regime should approximate "worst-case" conditions to provide the fullest protection against water quality violations, any conditions, however conservative, can be exceeded with some (possibly very small) frequency or probability. To plan to control events which occur on the average only once in a thousand years, say, would be to incur inordinate expenses. Thus, the selected flow regime must be in a sense an arbitrary design condition, corresponding to flow magnitudes which are adequate for design purposes a large majority of the time.

Waste load dilutions are, in Western Washington areas, lowest during summer low-flow conditions. The seven-day/ten-year low-flow conditions have been specified[2] for the State of Washington. These were determined for many points on streams around the basin using available U.S.G.S. data, and a set of streamflow analysis and synthesis programs (see Reference 1 for details).

Pollutant concentrations may be even greater, however, when materials which have accumulated on urban and agricultural areas over a dry period are washed off by a summer storm. Storms during the summer months are very common in the Pacific Northwest. Storm occurrence averages at least three measurable storms every summer. Due to this relatively high frequency of storms, runoff of non-point pollutants can be expected to occur during the worst-case design conditions.

The design storm selected for the purposes of including non-point runoff was a typical summer storm. It was assumed to have occurred after twelve dry days, which, based on historical data, was found to be the average period between summer storms. Runoff resulting from the average summer storm was input as a uniform flow over the 24 hour modeling period in the upper basins. A runoff pollutograph resulting from the storm was used in the Snohomish Estuary.

In addition to the above conditions, for the estuary a tidal condition corresponding to the typical monthly low swing was incorporated into the flow regime. This provided a conservative estimate of tidal flushing.

Because of the somewhat arbitrary nature of this flow regime, the above-mentioned flow conditions were presented for consideration to the Snohomish County Advisory Committee, and they were accepted.

Determination of Alternatives

Considerations included in the selection of alternative wastewater treatment configurations for the basins were:

- Locations of existing treatment plants;
- Suitability of existing facilities;
- Probable locations of future treatment plants;
- Optional locations for outfalls;
- Types of treatment plants, including storage facilities;
- Spatial distribution, and relationship to river and estuary system;
- Topography; and
- Soil conditions.

In developing alteratives, at all times only systems that would be hydraulically sound and that showed a potential to be simple, least cost, and reliable, were considered. To accomplish this, gravity systems were used whenever possible.

The list of alternative treatment plant and outfall locations, and types of treatment, for possible inclusion in the alternative plans was derived from previous studies, from discussions with local treatment plant operators, engineers and elected officials, and from the personal familiarity of Snohomish County Staff members. The alternatives chosen represent those most likely to be effective, based on the best engineering judgment of these sources and current EPA cost-effectiveness guidelines.[3]

Alternative configurations involving the possible combination of industrial and municipal flows were not considered acceptable when the industrial flows would be greater than about one-third of the municipal flows. This was due to the fact that the biological processes involved in treatment plants need a reasonably steady wastewater quality; this characteristic of municipal wastewater is easily upset by flow and quality variations in effluents from industrial sources beyond the control of the municipal treatment plant. The alternative of industry responsibility for the operation of the "combination" treatment plant was not considered at this time to be desirable.

The general objective of the various regionalized configurations was to achieve overall cost reductions through the economies of scale obtained from combining several local wastewater treatment plants. The additional costs of required interceptor sewers and/or force mains were included.

Wasteload Allocation

The execution of a cost-effective waste load allocation in the river basins required consideration of different types of sources (point, drainage district, and non-point), different time horizons with their varying water quality standards required by law, different receiving waters (rivers, estuary) and alternative regionalization schemes for wastewater treatment facilities. Many of these were interdependent.

In order to approach the identification of a most cost-effective basin configuration in an organized and effective manner, a working procedure was developed in advance of undertaking the task. This procedure is summarized in Figure 2 (supplemented by Table 1), which outlines the alternative "routes" which were considered demanding of investigation, in some cases conditional upon the findings from earlier phases. The following assumptions were used in this procedure:

1. Straightforward structural solutions were to be attempted first. Only if they were found unsuccessful would non-structural solutions be considered.

2. Where regionalized treatment plants were expanded existing plants, the same outfall locations would be used.

Assimilation Analysis

A very large number of computations are needed to determine water quality levels which result from a variety of wasteloads with complex hydrodynamic and natural constituent processes. Therefore, computer modeling of receiving waters for the analyses of waste assimilation was selected as appropriate. Computer modeling also allows rapid recomputation for various alternative cases, once the basic model has been established, thus facilitating comparisons.

The water quality computer models may also be used to investigate which estuary and river segments are "water quality limited," and which are "effluent limited".[4] Given conditions where all point sources just meet effluent standards, the former designation applies where receiving water standards are violated and the latter applies where they are met.

Waste Load Forecasts

In addition to specifying the receiving water geometry and the design flow regime, the water quality models require, as input, data on waste loads. Waste loads may, now or in the future, be directly subject to effluent standards, and may also be limited, indirectly, by receiving water quality standards. The objective of an assimilation analysis is to determine what may be discharged where, and yet meet the various pertinent standards.

Federal guidelines for effluent standards for municipal and industrial wastewaters have been, or are in the process of being, established. The standards become more stringent with time, varying in requirement from the "best practicable control technology currently available" or secondary treatment, to the "best available technology economically achieveable" or "zero discharge."

Proposed EPA standards for many industrial effluents are published in the Federal Register.[5,6] For each quality constituent, two effluent limitations are provided: (1) a maximum for any one day, and (2) a maximum average of daily values for any period of thirty consecutive days. The latter lower value was selected as the basis for computing industrial waste loads, since use of the former would be compounding worst-case events having a very small joint probability of occurrence.

The pollutant concentrations employed in the models as existing in effluent from secondary treatment in municipal wastewater treatment plants are given in Table 2. Where these values were uncertain, they were chosen to err on the high side, so as to provide a "worst-case" safety margin. Chlorine in secondary municipal effluent was modeled as a conservative (non-decaying) constituent. The various representative types and levels of secondary treatment employed in this study included:

- Oxidation Process (aerated ponds or ditches with 3 to 4 days retention capacity and effluent chlorination) meeting secondary standards (assumed maximum flow capacity of 2 mgd).
- High Rate Trickling Filters (primary sedimentation, H.R. filters with recirculation, secondary clarification, effluent chlorination).
- Conventional Activated Sludge (primary sedimentation, aeration, secondary clarification, effluent chlorination).

The municipal wastewater flows were predicted using a computer forecasting model, SNOQUAL, which determines flows on the basis of population dynamics. The details of this program are given in Reference 1.

One other important potential source of pollution is storm runoff from urban areas (in storm or combined sewers) or from agricultural lands (non-point sources). The manner in which these were computed and input to the models is discussed in Reference 1.

Rivers. A steady-state river water quality model (SNOSCI) as described in Reference 1, a specially modified version of DOSAG, was used for the river assimilation analysis. Numerous runs were made to test various boundary conditions. These consisted of point sources (municipal and industrial), non-point sources (agricultural runoff), and tributary streams.

The scheme of Figure 2 was used as a guide for running the alternative test conditions. First, runs were made with (a) zero point loads (representing 100% treatment) and full non-point loads, and (b) vice-versa. Point source treatment would be achieved by traditional structural means (sources and treatment plants); non-point "treatment" would be effected (at least partially) by "non-structural" measures such as by restricted land use and agricultural practices.

Next, with secondary treatment of municipal and industrial point sources, a number of runs were required to identify the locations and sizes required for reductions in non-point sources in order to meet receiving water quality standards.

The effects of various regionalized wastewater treatment schemes were then investigated, combining municipal and industrial effluents at certain appropriate outfall locations.

These investigations were repeated for present, 1980 and year 2000 waste flows.

Estuary. The transient estuary water quality model (SRMSCI) as described, in Reference 1, a specially modified version of RECEIV, for this study, and previously calibrated to the extent possible, was used for the estuary assimilation analysis. The design flow conditions included river inputs as per the output from the river model.

Numerous runs were made to test alternative municipal and industrial treatment schemes, again using the scheme of Figure 2 as a guide. An additional category of source, the Drainage District (treatable "non-point"), was included to represent two such extensive areas.

First, runs were made with no storm and non-point sources, and with point sources at secondary treatment. Next, the storm and non-point sources were included in the estuary model, and a number of runs were required to determine the locations and magnitudes of coliform reductions required to meet standards.

The "most stringent" regionalization scheme for the lower basin was run, with year 2000 municipal and industrial loads. This included municipal flows from Seven Lakes, Tulalip, Marysville, Lake Stevens, Mukilteo and Everett, all given secondary treatment at the present Everett Site.

Cost of Alternatives

The objective of these alternative costing procedures was to develop appropriate procedures for estimating costs for the large number of plan alternatives considered, each with its numerous facility components and with time phasing.

A computer model, SUSCI2, was developed by Systems Control, Inc., to design, time-phase, and cost sewers, force mains, pumping stations, and treatment plants. More details of this model are provided in Reference 1.

Given the alternative sewer networks, and locations and types of treatment plants, together with the forecast flows, SUSCI2 designs the facilities needed and computes the capital and M&O expenditures required, indicates the timing of costs over the planning period (1976-2000), and also determines a discounted total cost (present worth) for each alternative scheme. All the alternatives were costed with this model, taking advantage of common components (typically local sewer systems) which need not be repeated. Care was taken to ensure that the same total area was serviced under each alternative, regardless of the manner of servicing.

After making preliminary investigations into comparative costs of minor local alternatives, it was determined to be most efficient to analyze and select from the major alternatives first, then proceed to the intermediate and finally to the outermost and most minor and localized alternatives. The lesser costing alternatives were thus considered as variations of the preferable major (central) alternative. This approach was acceptable, since the effects of the minor alternatives were relatively small enough not to affect the selection between the major alternatives; this results principally from the fact that a small change in treatment capacity has less effect on the unit cost of treatment in larger plants than it does in smaller plants. As a result of this procedure, large numbers of cost evaluations of unattractive alternative combinations were avoided.

Costs for the chlorination of drainage waters in controllable drainage districts were computed manually.

The capital cost of a contact tank and chemical feed equipment was based on a formula by Smith[8] assuming dosage at 8 mg/L with a 15 minute contact time, and updating this to a 1976 dollar cost with an ENR Construction Cost Index curve for Seattle[9]. The M&O cost for chlorine, etc., was derived from a cost curve of operating costs of sewage tanks, after Engineering Science Inc., and making allowances for the recent large cost increases experienced for chlorine.

Cost-Effectiveness Comparisons

Alternative plans which met receiving water standards, as determined by the assimilation analysis, were compared for cost and effectiveness. Besides comparing the total discounted costs, their components (e.g., M&O vs. capital) were compared, since the M&O costs contained more uncertainty than the capital costs. Under effectiveness, such factors as reliability were considered. Thus, among schemes of similar costs, those with more force mains were less attractive than those with fewer (more reliable gravity sewers). If the differences in cost and effectiveness between two schemes was not sufficiently great, no preference between them was expressed on those grounds alone, and more detailed engineering would be necessary to determine the less expensive alternative. Differences between environmental impacts of alternatives were also considered.

Time-Phased Facility Schedule

A time-phased facility construction schedule, required to satisfy the demands of the basin management plan selected for the two basins, had to be determined.

As part of the assimilation analysis the receiving water quality models SNOSCI and SRMSCI, for the upper and lower portions of the basins respectively, were applied to investigate a number of alternative cases (see Figure 2). Computer runs for the projected year 2000 point loads treated at the secondary level determined that generally no problems occurred in the receiving waters, besides those due to non-point sources. Therefore, a schedule for the additional facilities required by the plan was simply, and practically automatically, governed by (1) the extra facilities needed by the year 2000, and (2) the dates when demands would exceed the capacities of existing facilities, or when the useful lives of existing facilities would expire.

The scheduling of facilities expansions was computed by the sewerage system planning and costing model named SUSCI2. Given the alternative sewer networks and locations and types of treatment plants, together with the forecast sewage flows, SUSCI2 designs the facilities needed and computes the capital and M&O expenditures required, indicates the timing of costs over the planning period (1976-2000, in four-year incremental planning periods), and also determines a discounted total cost for each scheme. Besides determining the needs for new facilities, SUSCI2 also computes extensions and updates needed to augment existing facilities; based on present capabilities, it estimates from input demand forecasts the dates when capacities will become inadequate. Since the designs are automatically optimized with respect to cost within SUSCI2, the results are automatically the most cost-effective.

The resulting time-phased development schedule was presented at local public meetings and at the technical advisory meetings. These meetings were specifically set up to enable the provision of practical inputs to plan scheduling.

The allocation of cost data over the implementation schedule was done by preparing the schedule in table form, and indicating therein the distribution of costs over the various incremental planning periods.

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Table 1. Types of Sources Included in the Four Cases of Figure 2

		Types of Sources Present		
		PTS	DD	NP*
Case	Segment Location	Point	Treatable Non-Point (Drainage Districts)	Elusive (Non-Treatable) Non-Point
1	Above DD's	Y	N	N
2	Below DD's	Y	Y	N
3	Below DD's	Y	Y	Y
4	Above DD's	Y	N	Y

*Partially treatable by non-structural means.

Definitions (also for Figure 2):

AWT - Advanced Wastewater Treatment
DD - Drainage District. These are agricultural areas where rain runoff is routed through systems of drainage ditches to adjacent rivers.
HPT - Highest Practicable Treatment
NP - Non Point Sources
PTS - Point Sources
2° - Secondard (Treatment)
Y - Yes
N - No

Table 2. Concentrations Resulting from Secondary Treatment of Municipal Wastewater, as Employed in Receiving Water Quality Models

Constituent	Concentration
BOD	30.0 mg/L
DO	5.0 mg/L
NH_3-N	9.8 mg/L
NO_2-N	0.0 mg/L
NO_3-N	10.0 mg/L
O-PO_4-P	10.0 mg/L
Cl_2	1.0 mg/L
Cu	1.0 mg/L
Pb	0.05 mg/L
Fecal Coli	200 MPN/100 mL
Total Coli	2000 MPN/100 mL
Temperature	25°C

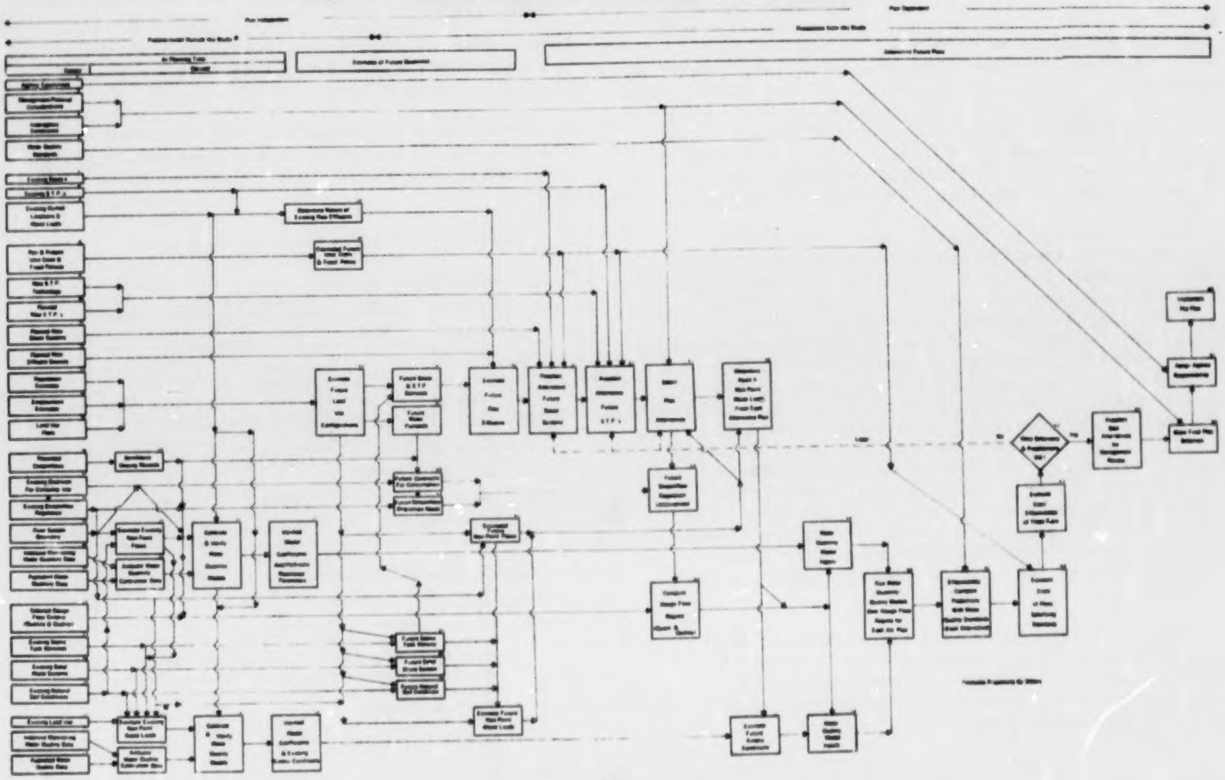
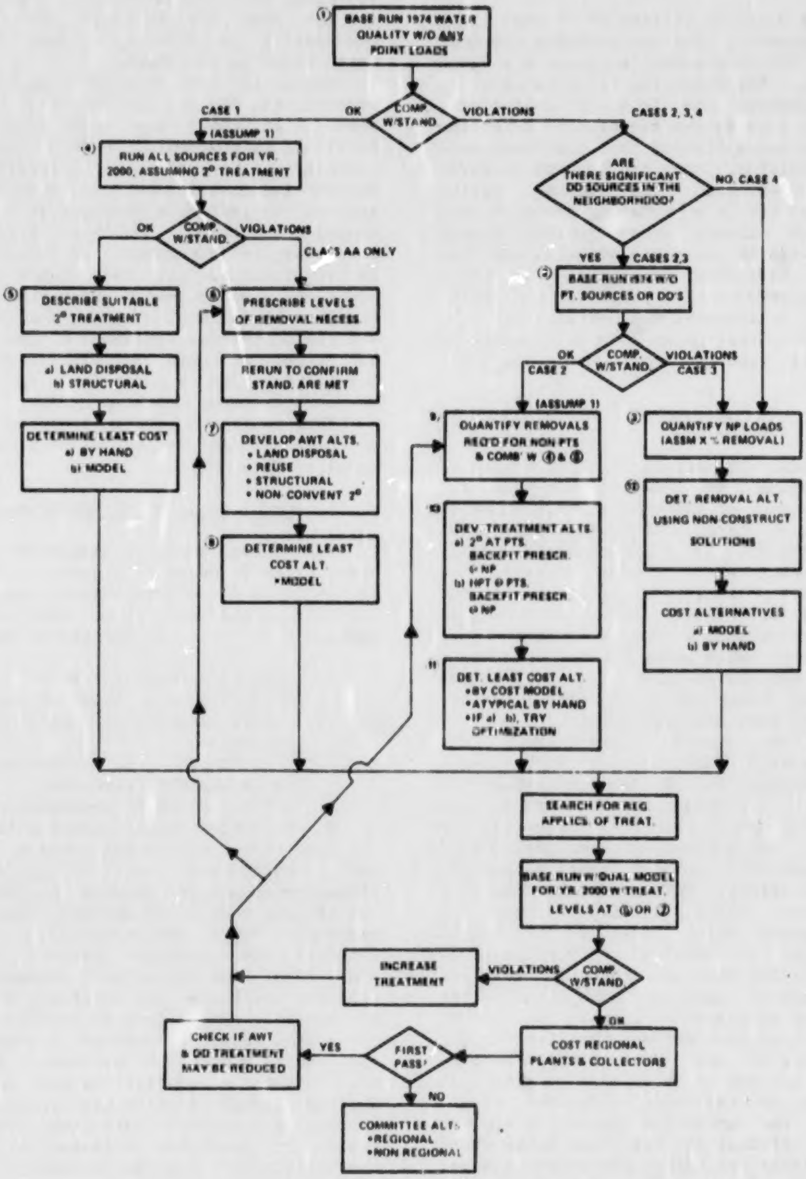


Figure 1. **WATER QUALITY MANAGEMENT PLANNING**

FIGURE 2

SCHEME FOR DEVELOPMENT OF ALTERNATIVES



①
BASE RUN 1974 WATER QUALITY W/O ANY POINT LOADS
COMP W/STAND
OK
CASE 1
VIOLATIONS
CASES 2, 3, 4
(ASSUMP 1)
④
RUN ALL SOURCES FOR YR. 2000, ASSUMING 2° TREATMENT
COMP. W/STAND.
OK
VIOLATIONS
CLASS AA ONLY
⑤
DESCRIBE SUITABLE 2° TREATMENT
a) LAND DISPOSAL
b) STRUCTURAL
DETERMINE LEAST COST
a) BY HAND
b) MODEL
⑥
PRESCRIBE LEVELS OF REMOVAL NECESS.
RERUN TO CONFIRM STAND. ARE MET
⑦
DEVELOP AWT ALTS.
• LAND DISPOSAL
• REUSE
• STRUCTURAL
• NON CONVENT 2°
⑧
DETERMINE LEAST COST ALT.
•MODEL
ARE THERE SIGNIFICANT DO SOURCES IN THE NEIGHBORHOOD?
NO. CASE 4
YES
CASES 2,3
②
BASE RUN 1974 W/O PT. SOURCES OR DO'S
COMP. W/STAND.
OK
CASE 2
VIOLATIONS
CASE 3
(ASSUMP 1)
9,
QUANTIFY REMOVALS REQ'D FOR NON PTS & COMB' W ④ & ⑤
10
DEV. TREATMENT ALTS.
a) 2° AT PTS.
BACKFIT PRESCR.
@ NP
b) HPT @ PTS.
BACKFIT PRESCR.
@ NP
11
DET. LEAST COST ALT.
•BY COST MODEL
•ATYPICAL BY HAND
•IF a) b), TRY OPTIMIZATION
③
QUANTIFY NP LOADS (ASSM X % REMOVAL)
⑪
DET. REMOVAL ALT. USING NON CONSTRUCT SOLUTIONS
COST ALTERNATIVES
a) MODEL
b) BY HAND
SEARCH FOR REG APPLICS. OF TREAT.
BASE RUN W/QUAL MODEL FOR YR. 2000 W/TREAT. LEVELS AT ⑥ OR ⑦
COMP. W/STAND.
VIOLATIONS
INCREASE TREATMENT
OK
COST REGIONAL PLANTS & COLLECTORS
FIRST PASS?
YES
CHECK IF AWT & DO TREATMENT MAY BE REDUCED
NO
COMMITTEE ALTS.
•REGIONAL
•NON REGIONAL

A REVIEW OF EPA'S GREAT LAKES MODELING PROGRAM

W.L. Richardson
U.S. Environmental Protection Agency
Large Lakes Research Station
Grosse Ile, Michigan

N.A. Thomas
U.S. Environmental Protection Agency
Large Lakes Research Station
Grosse Ile, Michigan

Summary

The Large Lakes Research Station at Grosse Ile, Michigan, is responsible for implementing the EPA, Office of Research and Development's research program for the Great Lakes. The objective is to be able to describe the transport and fate of pollutants. Mathematical models provide the researcher with the necessary tools for accomplishing this task and, once calibrated and verified, they can be used by water quality managers confronted with making policy decisions. Several levels of modeling research have been initiated which address water quality issues ranging from lake-wide to nearshore effects, and from eutrophication to hazardous materials. Concurrent surveillance and experimentation programs are being conducted for model calibration and verification. An overview of the EPA Great Lakes modeling program is presented including results from some specific models.

Introduction

The Environmental Protection Agency, Office of Research and Development, is conducting a research program to address many of the complex water quality issues on the Great Lakes. The Federal Water Pollution Control Act and the 1972 Amendments[1] specify that the agency ... "shall conduct research and technical development . . . with respect to the quality of waters of the Great Lakes, including an analysis of the present and projected future water quality of the Great Lakes under varying conditions of waste treatment and disposal." The U.S.-Canada Agreement on Great Lakes Water Quality[2] further provides impetus for this research effort.

In response to these directives, the Environmental Research Laboratory--Duluth, Large Lakes Reasearch Station (LLRS) is implementing a modeling research program to improve the understanding of complex limnological processes in the Great Lakes. The program has been implemented primarily through grants to academic institutions and by a small in-house effort. This research dovetails with a concurrent water quality survey and experimentation program which provides information necessary for model calibration and verification. The models are providing decision makers in EPA and other water management agencies with quantitative tools for evaluating alternative courses of action concerning water quality. Because the limnological processes are so complex and interrelated; because the Great Lakes include such a large geographical area; and because of the long detention times; simple, empirical and intuitive approaches are not adequate. This is critical for the Great Lakes where billion dollar decisons can affect the entire system. Though the cost of modeling one Great Lake may be on the order of a million dollars, the billions spent for remedial actions justifies the effort. As a model for each of the lakes is developed, less data and experimentation are required which reduces the cost of each subsequent lake modeling program. In addition, the model structure, kinetics, and software can be used for smaller lakes which would not necessarily be modeled without having the Great Lakes modeling experience.

Models are not expected to answer every question, however, and the researchers would be the first to agree that there are major deficiencies which are difficult to overcome. These include the imprecise scientific knowledge of specific processes and interactions and further computational restrictions imposed by available computer technology and cost of computer operation. Models are intended to enhance the managers' experience and judgement and improve their insight into cause and effect. In addition, the modeling research provides secondary benefits by (1) systematizing and quantifying complex interrelationships between the physical, chemical and biological elements in limnology and (2) by identifying the weakest areas in our knowledge and, in fact, defining research needs.

This paper presents an overview of the general modeling process along with a summary of specific model results.

Great Lakes Model-Management Process

The general modeling-management process for the Great Lakes is shown in Figure 1. Modeling is the focus for understanding limnological processes and for translating them into terms necessary for management's use. The process as shown includes:

1. Monitoring material inputs.
2. Surveillance of material pools.
3. Experimentation to define biochemical processes.
4. Establishment and management of water quality standards.
5. Establishment of abatement programs.
6. Action to reduce material loads.

Development of a model entails both calibration and verification. Calibrating a model involves comparing computed results to measured data and adjusting model parameters until the computed variables match the measured. Verification is obtained when computed results match data from an independent data set without parameter adjustment.

Once calibrated and verified, the model is used to simulate the effect of possible modifications to the system (e.g., reductions in phosphorus loads) on the concentration of materials in the water body. The simulated concentrations are compared to those desired (water quality standards). The results can be used as a basis to establish long-range planning goals, to determine effluent allocations, or to reestablish water quality standards.

Model Development

Water quality models are structured to predict the effect of material discharges (loads) on material concentrations in the receiving water body. Two modeling approaches are in general use. They are 1) empirical and 2) deterministic. The empirical or statistical approach involves correlations of cause factors to effect factors. For example, Vollenweider[3] has compiled total phosphorus loading data on several lake systems and correlated these to the measured peak chlorophyll a levels. Since a range of conditions has been incorporated, predictions of the effect of phosphorus reductions are made by interpolation.

The disadvantage of this approach is that there are several assumptions which may limit its use particularly for the Great Lakes: 1) it assumes the phosphorus loadings are known and correct, 2) it assumes the chlorophyll a is in equilibrium with the loads (ie., there is no time lag in response to the loads), and 3) it assumes average conditions are sufficiently precise.

The deterministic approach is based on basic principles and incorporates equations representing the actual limnological processes. These models account for and trace each variable through the system and conserve mass, energy, and momentum in space and time.

For the deterministic models the calibration or data "fitting" process is based on knowledge of the system parameters in contrast to the empirical approach which forces a least squares fit to the data. If the deterministic model output from initial simulations does not match the data, a limnological rationale for parameter adjustment is necessary. If a rationale is not available then further experimentation is required. Any interim results are qualified to reflect the range of possible solutions. The disadvantage of the deterministic approach, however, is that it requires much more research time and computer resources.

The modeling process includes, but is not necessarily limited to, the following steps:

A. Assessment Phase
  1. Define issues.
  2. Define objectives.
  3. Conceptualize model.
  4. Assess general data availability.
  5. Determine capabilities and requirements of various model approaches.
    b. Assess model accuracy.
    a. Describe information the model can provide.
    c. Determine time required to develop and implement.
    d. Determine computer resources required.
B. Decision Phase
  1. Determine resources available.
    a. Computer time.
    b. Research resources.
  2. Determine priorities.
  3. Determine accuracy required.
  4. Determine deadline.
  5. Choose a course of action based on the above assessments.
C. Implementation Phase
  1. Develop and implement model.
  2. Compile existing data.
  3. Design and implement surveillance and experimental programs.
  4. Calibrate model.
  5. Determine success of approach and modify accordingly.
  6. Verify model.
  7. Evaluate the success of the model.
  8. Present results to the scientific community.
  9. Document models.
D. Management Phase
  1. Conduct management simulations.
  2. Make model available for management use.
  3. Modify and refine model as required.

Great Lakes Issues

The issues concerning the Great Lakes can be categorized by water quality parameters and the time and space scales involved. The most urgent issue is eutrophication. The problem is the effect of phosphorus and nitrogen on levels of algal biomass and the degree of control required to restore and/or maintain adequate water quality. This issue requires knowledge of lake-wide phenomena and even phenomena involving the interaction between lakes. The time scale is on the order of years to decades.

A second level issue also involves eutrophication but in the nearshore regions and embayments. Because of the shorter response time in these localized areas, time and space scales are smaller (seasons and kilometers).

A third level issue involves immediate effects on even smaller scales (hours and meters) of materials or heat in the discharge plume. For example, the material distribution in an effluent plume may be critical to nearby water intakes or recreational sites. Specific questions have been asked such as Where to locate the discharge structure? What size mixing zone is allowed so not to interfere with water uses? and What local and short-lived biological responses are expected?

Great Lakes Models

General

The first phase in modeling each of the Great Lakes (except Superior) involves development, calibration and verification of the phytoplankton-zooplankton-nutrient model first structured by O'Connor[4], for the San Joaquin Delta.
The general system scheme of this approach is depicted in Figure 2.

Phytoplankton biomass is represented by chlorophyll a which is used primarily because of the ease of measurement and availability of data. Phytoplankton carbon is obtained by specifying a carbon-chlorophyll stoichiometry and is the element zooplankton consume along with the nutrients contained in the phytoplankton. The nutrients, phosphorus and nitrogen are also accounted for and traced through the phytoplankton and zooplankton by specifying stoichiometry relationships with carbon. Phytoplankton growth rate is a function of temperature, light, and nutrients and follows Michaelis-Menten product kenetics. The model includes nutrient recycling, phytoplankton settling, nutrient sedimentation, and material loadings. Because of the large time and space scales involved, the lake is represented by a few segments, each assumed to be homogeneous. The model output respresents the average concentration in each segment.

Lake Ontario

Lake Ontario was the first Great Lake to be modeled using this approach. This was initiated for the International Field Year on the Great Lakes (IFYGL) by a grant to Manhattan College. This work culminated in a two volume EPA Ecological Research Series Report[5,6]. In summary, the Lake Ontario effort involved the calibration of the phytoplankton/nutrient structure for the three layer segmentation scheme (Lake-1) shown in Figure 3. The results have been reported to the International Joint Commission (IJC) for management considerations.

The results, depicted in Figure 4, indicate that the chlorophyll a levels are not in equilibrium with the nutrient loads. This is evident because the simulated peak chlorophyll *a* continues to increase for about 6 to 8 years before reaching an equilibrium level. Further, even with reducing the phosphorus loads to levels set by the Water Quality Agreement, chlorophyll *a* levels are predicted to increase to a new equilibrium.

With Lake-1 having been substantially calibrated, work continues at Manhattan College to refine the Lake Ontario model by 1) addition of spacial detail (Figure 5); and, 2) addition of biological detail (multi-species). The limiting factors in this work are not the expansion of the model structure itself, but with data availability and the overwhelming task of data reduction for model verification. In addition, there is the matter of interpreting model output. The analyst soon becomes overwhelmed by the reams of computer output even if these have been reduced to graphical form. To overcome these limitations, the model researchers have been relying to a great extent on the EPA STORET system for data archiving, manipulation, and statistical analysis. Also, more work is underway to output both data and model computations in graphical form. The Manhattan College staff has even produced movies of model ouput to reduce the effort in interpreting their results. Research is now proceeding with the development of statistical techniques to determine how well these complex models represent the data.

Lake Huron

The Lake Huron modeling effort is also being conducted by Manhattan College under the direction of the EPA Large Lakes Research program. The modeling research is being conducted in conjunction with the IJC Upper Lakes Reference Study and the results will have direct input to this management level report.

Essentially, the same model structure is being applied with a 5-segment scheme shown in Figure 6. The unique aspect of this system is the high material gradients evident in and extending from Saginaw Bay. This is an excellent case to test the general applicability of this model structure.

Lake Erie

The Lake Erie eutrophication model includes similar nutrient-biological systems applied to a 5-segment scheme (Figure 7) except that the process of dissolved oxygen depletion and resulting nutrient regeneration must be incorporated. Manhattan College is progressing with this task while concurrent field effort is being conducted by Ohio State University and State University College of New York at Buffalo.

Lake Erie is also the site of an issue involving the effect of power plants on fish populations. To address this issue a research program has been initiated involving both data collection and model development for fish in the western basin. The model will incorporate data collected on the number of fish larvae passing through a power plant and the number observed in the western basin. The effect on the adult populations in time will be computed.

Saginaw Bay

Modeling research on Saginaw Bay, Lake Huron, is being conducted by the LLRS at Grosse Ile. Eutrophication is the primary issue in Saginaw Bay evidenced by the highest chlorophyll *a* levels recorded in the Great Lakes system. A sub-issue is the effect of blue-green algae on taste and odor in municipal water supplies.

Two parallel modeling efforts are progressing. First, the Manhattan model structure is being applied to a five segment scheme[7]. This application research has benefitted the program by not only providing insight into cause and effect but also by familiarizing EPA personnel with the details of the Manhattan models and computer programs. This has enhanced relationships with the grantee and has resulted in better program management. In this way, the LLRS has or will have the capability of operating any of the models developed by Manhattan College.

The second in-house modeling effort on Saginaw Bay involves development of the next generation of verified ecosystem models. Bierman[8] has structured a four class phytoplankton model which includes more detailed interaction kinetics in place of Michaelis-Menten kinetics. Model results are being used in the IJC Upper Lakes Reference Study report.

The Saginaw Bay modeling research is also being expanded to include the fate and transport of hazardous materials. A preliminary model structure is being formulated and surveillance and experimental research is being implemented.

Transport Models

Another modeling effort being conducted with support of the LLRS is devoted to describing the detailed transport processes in the Great Lakes. The primary objective is to develop a general approach to describing pollutant transport on relatively fine time and space scale in the near-shore region. The work is being done at Case Western Reserve University[9].

The models use the first principle conservation equations for mass, momentum, and energy. Winds and solar radiation drive these equations which result in computed current velocities, current direction, and thermal structure in three dimensions. Verification of this type model is difficult and requires synoptic data at many points. The application is being demonstrated along the Lake Erie shore near Cleveland and will describe the course of the Cuyahoga River discharge into the lake.

The transport models are also being used to evaluate the potential effect of the proposed Cleveland Jetport on water quality and temperature structure. By varying the model geometry to represent the proposed configuration of the jetport, it is possible to predict the circulation patterns and the subsequent distribution of material concentrations (Figure 8).

Using the same general approach, Paul[10] has developed thermal plume models which have been substantially verified at the Point Beach Power Plant on Lake Michigan.

Conclusions

The experience gained thus far in implementing the Great Lakes modeling effort has led to a number of conclusions which may be helpful to others initiating similar modeling programs.

First, the structuring and calibrating of a model derives benefits long before a final verified model is obtained. The modeling process requires a systematic approach to data collection and analysis. Intermim results reveal gaps in knowledge for a particular system or process and are useful in defining and directing new study and research.

Second, most of the effort in the modeling process is involved with data reduction. Relatively, little effort is required to generate reams of theoretical computer output. The primary concern is to structure a model with sufficient bio-chemical detail to be realistic, but simple enough so as not to be data limited.

Third, considerable effort is required to calibrate and verify large scale models even with existing model structure and computer programs. For this reason, this process appears to be in the realm of applied research rather than engineering application. A modeling program of necessity should not be separated from a total research program. This program involves the entire range of model structuring, experimentation, and research surveillance.

Finally, because of the resource commitments made to the total research effort, once a model has been implemented, i.e., calibrated and verified, a continuing effort should be made to document the model, and to keep it operational. In this manner, models could be used to assist in answering the many short-term, day-to-day questions facing the EPA and other environmental regulatory agencies. Only after calibration and verification for a specific system can a model be turned over to an engineering staff for general management application.

One continuing question remains, however, and that concerns the confidence placed on model results by managers. Progress in gaining managerial confidence is being made as more rigorous techniques are developed to evaluate how well model results match the data. In the final analysis confidence will come as model predictions accurately forecast actual water quality. For Saginaw Bay, with its short response time, verification data will soon be available to test predictions of the eutrophication models. A good fit there could go a long way toward convincing managers of the utility of the other Great Lakes models.

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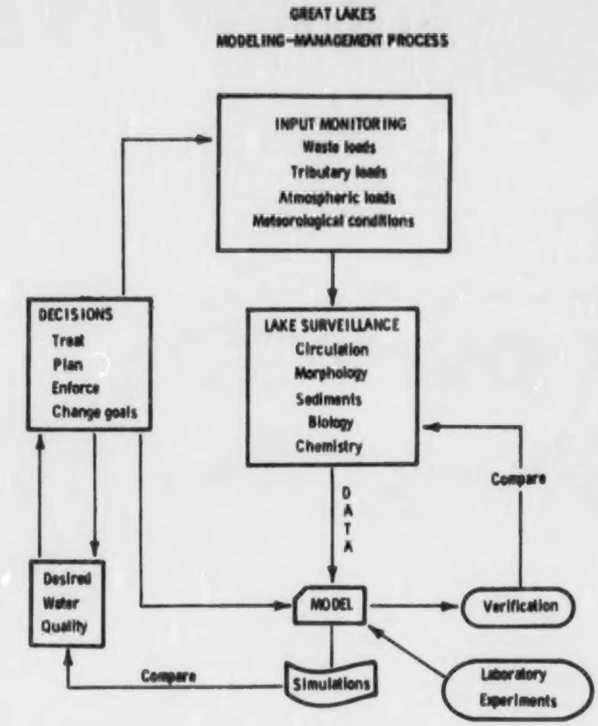
GREAT LAKES
MODELING–MANAGEMENT PROCESS
INPUT MONITORING
Waste loads
Tributary loads
Atmospheric loads
Meteorological conditions
DECISIONS
Treat
Plan
Enforce
Change goals
LAKE SURVEILLANCE
Circulation
Morphology
Sediments
Biology
Chemistry
D A T A
Compare
Desired
Water
Quality
MODEL
Verification
Compare
Simulations
Laboratory
Experiments

Figure 1. Great Lakes Model-Management Process.

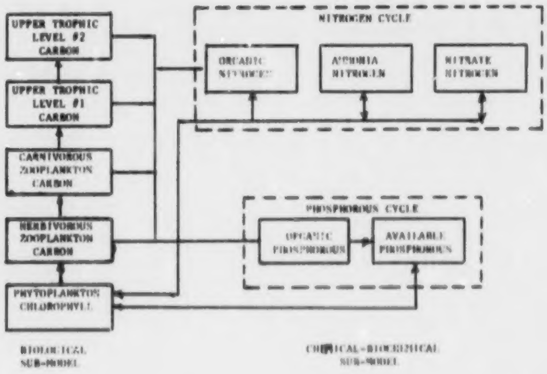
UPPER TROPHIC LEVEL #2 CARBON
UPPER TROPHIC LEVEL #1 CARBON
CARNIVOROUS ZOOPLANKTON CARBON
HERBIVOROUS ZOOPLANKTON CARBON
PHYTOPLANKTON CHLOROPHYLL
NITROGEN CYCLE
ORGANIC NITROGEN
AMMONIA NITROGEN
NITRATE NITROGEN
PHOSPHORUS CYCLE
ORGANIC PHOSPHORUS
AVAILABLE PHOSPHORUS
BIOLOGICAL SUB-MODEL
CHEMICAL-BIOCHEMICAL SUB-MODEL

Figure 2. General Eutrophication Model Structure[5].

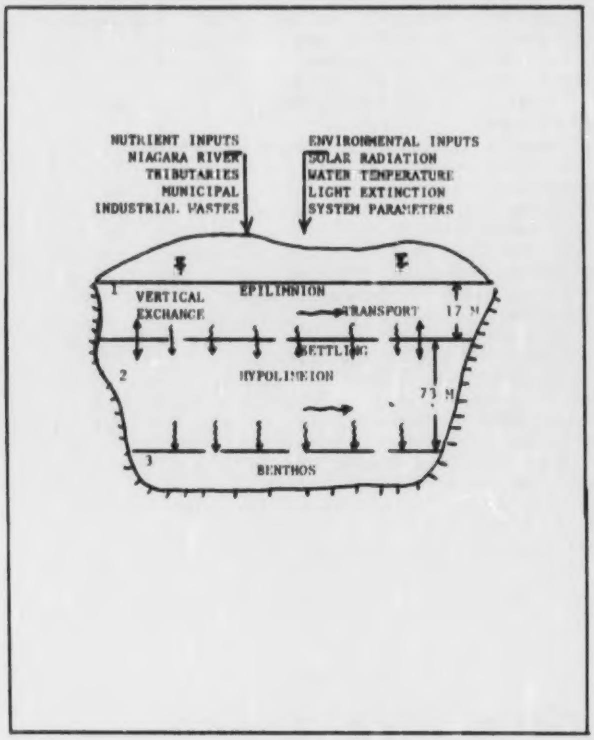
NUTRIENT INPUTS
NIAGARA RIVER
TRIBUTARIES
MUNICIPAL
INDUSTRIAL WASTES
ENVIRONMENTAL INPUTS
SOLAR RADIATION
WATER TEMPERATURE
LIGHT EXTINCTION
SYSTEM PARAMETERS
1
EPILIMNION
VERTICAL EXCHANGE
TRANSPORT
17 M
SETTLING
2
HYPOLIMNION
73 M
3
BENTHOS

Figure 3. Lake Ontario (Lake-1) Model Segmentation[5].

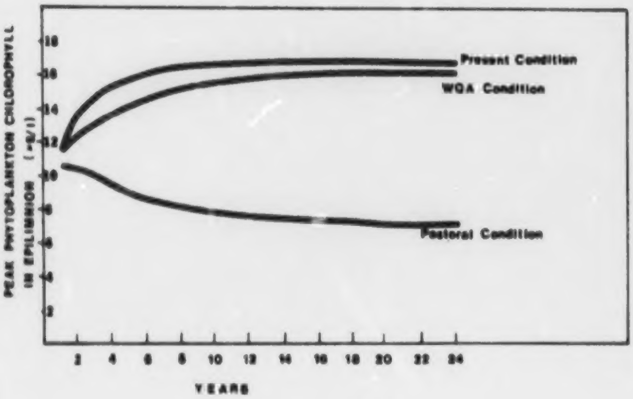

Figure 4. Projected Peak Clorophyll a Concentrations for Lake Ontario[6].

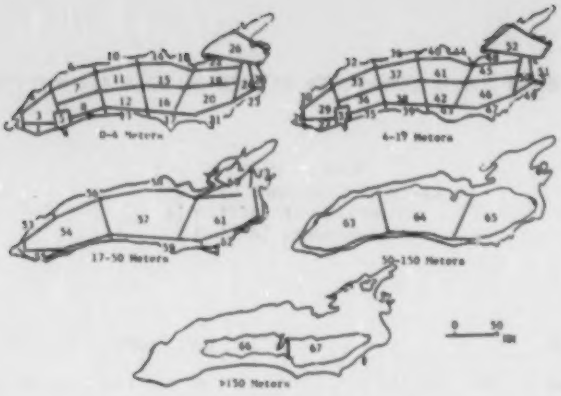
0-6 Meters
6-17 Meters
17-50 Meters
50-150 Meters
>150 Meters
54
57
61
63
64
65
66
67
0 50
km

Figure 5. Lake Ontario (Lake-3) Model Segmentation.[5]

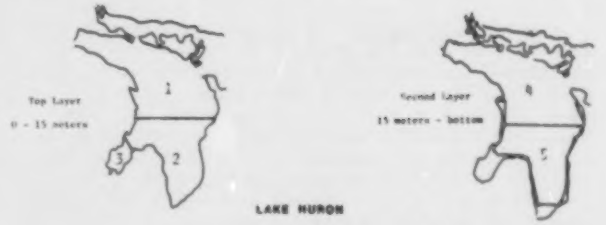
Top Layer
0 - 15 meters
1
2
3
Second Layer
15 meters - bottom
4
5
LAKE HURON

Figure 6. Lake Huron Model Segmentation.

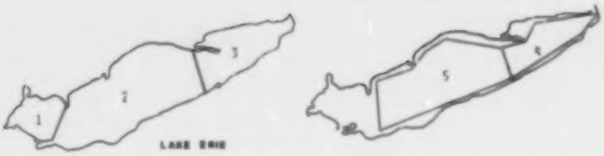
1
2
3
4
5
LAKE ERIE

Figure 7. Lake Erie Model Segmentation.

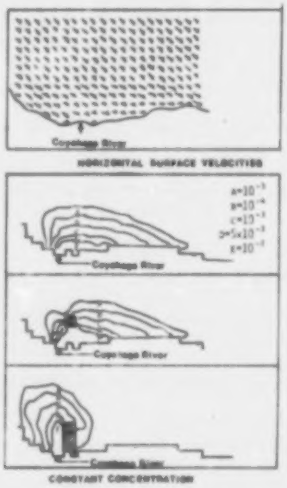

Figure 8. Simulated Currents and Conservative Material Concentrations for Alternative Jetport Configurations.

THE DEVELOPMENT AND IMPLEMENTATION OF USER ORIENTED AIR QUALITY MODELS

John J. Walton
Lawrence Livermore Laboratory
University of California
Livermore, CA 94550

Abstract

Implementation of the Clean Air Act and its amendments requires that decisions be made, at various levels of government, on many complex questions. In order to facilitate the work of decision- and policy-makers, readily useable air quality models must be developed. Such models can have quite different requirements and constraints than those developed primarily for research purposes. These needs will be identified and past experience will be drawn upon to illustrate how some of them have or have not been met.

Introduction

The National Science Foundation, through its Research Applied to National Needs (RANN) program, has sponsored an interagency program at the University of California Lawrence Livermore Laboratory (LLL), the NASA-Ames Research Center (ARC) and the Bay Area Air Pollution Control District (BAAPCD) to develop and validate a regional air pollution model which can be applied to the air quality problems of the San Francisco Bay Area. This work resulted in the Livermore Regional Air Quality (LIRAQ) model.[1,2] The model calculates in the two horizontal dimensions the transport, dispersion and chemical changes undergone by the most significant photochemically reactive and non-reactive air pollutants in the San Francisco Bay Area. Through the approximately three year duration of this project a wide variety of problems were encountered and handled with varying degrees of success. This experience has given us a feeling for the various, often interrelated, factors which must be considered by both user and modeler in order that an appropriate and useable air quality model be developed. It is our purpose here, to share our thoughts on this subject with the attendees of the EPA Conference on Modeling and Simulation.

Just as the atmosphere itself exhibits many complex and interrelated features, so does the process of user/modeler communication and compromise needed to cope with the diverse requirements and constraints governing model development. We have chosen to break these into three broad categories:

I. The needs of the user group or agency.

II. The inherent physical complexities and constraints of the specific problem.

III. The various resources which the user has at his disposal.

It should be emphasized that these are not independent factors and frequently compromises need be made between them. In the balance of this paper we will describe in more detail the various aspects of each of these factors.

I. User Needs

We see the user as any group or agency which may come to the modeler seeking to address questions related to air quality. The user's needs will provide the framework required for model development. Here we can identify five basic considerations, each one of which is related to some degree to the others.

Model Application. Unlike the modeler, for whom the model is a tool with which to explore the nature of pollution, its origins and evolution, the user will in general be charged with a specific responsibility and a model directed to this end will be required. Some examples of specific applications are: the study of pollution episodes, support in legal action, assessments required in land use planning, study of the efficacy of of various pollution abatement strategies and regulation needed to implement mandated standards. It should be pointed out, that while there may be overlap between several of these areas, an agency charged with more than one responsibility may, in fact, require more than one model.

Pollutant Characteristics. Depending upon the time and space scales of concern, the pollutants of interest may be anything from inert to highly reactive, or they may have properties which make them subject to specific scavenging processes. For example, nuclear releases are considered inert but may consist of particulates which will settle out at some known rate. Hydrogen sulfide, stored at a geothermal sight can, depending upon concentration, be anything from lethal gas to an unpleasant odor. Further, if the time scale of interest is of sufficient length (approximately one day) the gas will oxidize to produce sulfates which may precipitate out as an "acid rain". The pollutants associated with combustion range from effectively inert carbon monoxide to hydrocarbons and the oxides of nitrogen and sulfur which lead to the secondary pollutants ozone/oxidant and particulate sulfates. The effects may not be direct, for example, the Department of Transportation sponsored Climatic Impact Assessment Program (CIAP),[3] which, among other things considered, explored the effect of ozone reduction in the stratosphere, due to effluent from supersonic aircraft, upon ultraviolet radiation at the earth's surface.

Spatial Domain. The area of interest can be anything from the region immediately downwind from a power plant stack to the entire globe. Local models would, for example, be employed to treat processes going on in the vicinity of industrial facilities. The LIRAQ model mentioned above is concerned with regions of characteristic dimension of one-hundred to two-hundred kilometers. The question of the sulfate budget in the eastern United States would be of subcontinental proportions. Finally the CIAP project employed global models of one, two and three-dimensions. It should be clear that the size of the domain will influence the degree of spatial detail which can be achieved. Spatial domain relates also to vertical extent. Although it will depend strongly upon the application, we can say roughly that local and regional problems may be addressed with models focusing on a well mixed layer below an inversion, if it exists (less than a kilometre), subcontinental models may go through the convective cloud layer (three to four kilometres) and global models may be expected to extend into the stratosphere (thirty to thirty-five kilometres).

Temporal Scale. The time periods of interest may be anything from hours to years. As mentioned above, the time period treated by the model may influence those physical characteristics of the pollutants which must be emphasized in the model calculation. In turn, the time scales of interest are roughly related to the spatial domain under consideration extending from local problems simulating hours to global scales which may be concerned with processes evolving over periods of years.

Confidence Level. Any model, however complex, is only an approximation of physical reality. As will be discussed in the following sections of this paper, the modeler is limited in the number of processes which he can describe and even these are sometimes not fully understood or must be treated with approximations. The question then is, to what degree can the model be expected to reproduce the physical picture which is observed? Further, because of the demands put upon him, what degree of accuracy does the user need in order to make meaningful judgements? This criterion is frequently related to domain of interest. For local problems one might expect to achieve results with accuracy of ten percent while regional and subcontinental problems might be considered reliable when giving results within tens of percent. For global calculations, sometimes order of magnitude or even the sign of a change may be sufficient.

The user will, in general, have a well defined application, including the pollutants of interest, while temporal and spatial scales may be less specific. The modeler will be able to provide guidance in determining what confidence level can be realistically expected from model results. Communication between the user and the modeler is vital during this foundation stage of model development, in order that both parties be aware of and appreciate the various requirements and constraints and the compromises which must be made between them. The definition of possible constraints will lie primarily in the purview of the modeler and rests upon the second factor governing the model.

II. Physical Processes and Constraints

Under this heading the modeler must consider any process or condition, either natural or man-made which might contribute to the state of the physical system which he is trying to describe. He must always make compromises between what he would wish to treat and what lies within the capacity of the state-of-the-art or of his resources to handle. Discussed here are those factors which most commonly will play a part in the problem.

Sources. Man and nature both provide the atmosphere with effluents through a variety of sources. Some of the natural sources which contribute to our "ambient" atmosphere are; forests (hydrocarbons), soil micro-organisms (methane, nitrous oxide, hydrogen sulfide), fires (carbon monoxide and particulate), volcanoes (sulfur, fluorine, particulate, hydrochloric acid) and oceans (chlorides, calcium and sulphates). The pollutants we consider from man's activity are particulates and species such as carbon monoxide, hydrocarbons and oxides of nitrogen and sulfur resulting from combustion processes in transportation and power generation. In parts of the United States SO_2 from space heating is significant. By-products such as hydrogen sulfide, flourine, trace metals and volatile hydrocarbons from various industries may present problems in some areas. Pesticides form another class of pollutant which we may wish to follow, while industrial accidents and leaking storage vessels provide a whole spectrum of problems of local concern.

Chemistry. The above are considered primary pollutants and their reactions with other species present and their response to the diurnal solar cycle help to define the level of chemical complexity required in the model. If these pollutants alone are of interest it may be possible to treat their reactions with simple chemistry or decay terms. However, as mentioned earlier, depending upon time scale these may lead, through a chain of more complex reactions to secondary pollutants. Among these secondary pollutants are ozone or oxidant resulting from the presence of hydrocarbons and the oxides of nitrogen in the presence of sunlight. Similarly, oxides of sulfur lead to sulfate thence to sulfuric acid in the presence of water.

Meteorology. Here we mean all of the natural processes in the atmosphere which can affect the pollutants being considered. Turbulent winds will transport and disperse the pollutants. The presence of water vapor will promote heterogeneous transformation; water vapor in the form of clouds will affect photodissociation processes, while rainfall provides a mechanism for the scavenging of certain pollutants (e.g., sulfates and nitrates).

Radiation. As mentioned in the above sections, photochemical reactions may play a role in the problem and hence the significance of solar radiation transport. Generally, for models on scales less than global, radiation is a, possibly time-dependent, input quantity. It is however clear that feedback mechanisms may exist which can play a significant part in the evolution of the chemically active species and the radiation balance.

Topography. The character of the terrain in the region can affect, directly or indirectly, source input, chemistry and transport. For example, a source elevated due to the terrain may emit above an inversion, which will inhibit its transport to the surface. Surface characteristics can affect heating, modifying the chemistry and possible convective activity. Complex terrain such as that seen in the San Francisco Bay Area has strong channeling effects, giving rise to characteristic flow and pollution patterns. Finally, the character of the terrain will affect the level of turbulence and hence dispersion rate.

Boundary Conditions. Since there will usually be conditions outside the model domain which can affect what occurs within, a set of boundary conditions must be supplied to the model to account for these. These consist of pollutant background values, possible upwind sources and transport across the domain boundaries. As the model becomes more complex, more information will be required. Pollutant background is usually available from observations in unperturbed regions. Information on upwind sources may be more difficult to acquire, frequently being outside the region of influence of the user. Recourse must then be had to some, hopefully realistic, artiface. Transport at the domain boundaries is of course the mechanism by which conditions outside the region affect processes within. This information is generally available through the same process that provides wind fields for transport within the region.

Through this second stage the modeler has had to determine those physical characteristics and processes which are required to provide a model which will meet the user's needs. This is a phase during which actual numerical experiments will be carried out, in order to test new ideas and also to see if already existing programs or subprograms can be adapted to address the user's problem. There are, in fact, a number of "off-the-shelf" models of varying complexity which are available to the potential user and it is to be hoped that as the process of developing user oriented air quality models continues, readily adaptable programs will become increasingly available.

One might expect that once the model requirements have been defined and the pertinent physical processes identified it would simply be a matter of writing a computer program, handing it over to the user and going on to other things. However, anyone who has had to function within a budget will be well aware that further compromises must be made, because there never seems to be sufficient money to do all those things desired. This brings us to the final factor.

III. User Resources

Here we are concerned with any factor which may tend to facilitate or impede the process of addressing the user's problem. Here the user and modeler must work in concert to apply available funds in the most efficient way possible.

Computer Availability. User and modeler demands must be compatible with the available computational facilities. A computer offers, at a price, some degree of computational speed, a certain amount of storage for coding and data, and some form of input/output facilities. The modeler, in developing a large, complex program will be constrained by the size of the computer available although some tradeoffs between speed and storage are possible. The user, on the other hand, is more concerned about the speed with which the computer can run his problem and provide him with useable output. This question of "turn around" time depends to a certain extent upon the user's mission. A land use planner can afford to wait several days for his answers, while an agency which must respond to sudden emergencies will require immediate answers albeit, in less detail than those of the former. With a given computer system, the actual time (cost) involved in computation rests upon the model complexity. Compromise is almost invariably required between the modeler who wishes to include as much physics and chemistry as possible and the user who finally pays the bill.

Data Availability. User and modeler both are plagued by the lack of data and as more and more complex models are developed the need for data is correspondingly increased. We wish to have data for all physically pertinent aspects of our problem, at least over the domain of interest. Source data for the model are often not available at all from direct measurement and must be estimated from indirect measures such as population, industrial and traffic flow patterns. Meteorological data are generally sparse, entailing the use of various types of interpolative schemes to provide information over the entire domain. Pollutant data, required for model validation are often incomplete or difficult to measure with accuracy.

Response Time. There are two kinds of response time which concern the user and constrain the modeler. The first is the time available for model development. This is imposed upon the modeler by the user in order that the user may meet his commitments. As mentioned in Section II of this paper, there is an increasing number of existing air quality models which help to alleviate this problem. On the other hand, we tend to make increasing demands upon our models which involves the inclusion of more physical mechanisms and the use of more sophisticated numerical techniques. The second time constraint was alluded to in the first part of this section, that is the model/computer response time, which is imposed by the user's mission upon the computer choice and model design.

Personnel. Finally, in order that an air quality model be appropriate for a given problem and provide useable results, communication links must exist at all levels of development and application. In general, the responsibilities and background of user personnel will be quite different from those of the modeler. The modeler is expected to be aware of the relative importance of the many physical characteristics of the problem and how they may be addressed, while a local air quality agency, for example, may be expected to supply decision and policy makers with information pertaining to the impact of changing population patterns and pollution abatement strategies. As models become more complex, the user may find that a third party or model operator is required to provide direct operation of the model and to interpret its raw results.

During model development direct user/modeler links are necessary for the reasons mentioned earlier in this paper. They are: to reconcile the user requirements with the modeler's ability to produce a functional model within the constraints imposed by the physics and chemistry, data availability and computational facilities, and to make the user aware of the model's features and limitations. Once the problem has been defined, continued communication will help to keep the project on track to its desired goal. To this end there are several options available. First, formal and informal reports always have a place, particularly in providing documentation of the work in progress and of the model upon completion. They do not, however, provide very direct user/modeler interaction. In the LLL project a "user advocate" was employed to meet this need. This person is a member of the developer agency who acts as the user's representative with the modeling group. The role is demanding in that it requires not only a full knowledge of the user's needs but also a knowledge of the limitations under which the modeler must function. Perhaps the best approach, if it is economically feasible, is to have direct user participation in model development. Though the BAAPCD did not participate directly in the LIRAQ model development, they did play a major role in data acquisition.

The most important communication link is the last, that between the finished model and the user. The user should be able to formulate a problem in his own terms and have it executed. Computed results must then be provided to the user, again in his own terms. As an example of how this was achieved in one case we can use the LLL LIRAQ model. The name LIRAQ refers specifically to the air quality program itself. In order to facilitate the use of this model by the BAAPCD several other programs have been provided. The "Problem Formulator" is a program which provides an interface between the actual running code (LIRAQ) and the user. Through a series of questions to the user the Problem Formulator determines the type of problem to be run, physical conditions, spatial domain, etc. This in turn provides a series of instructions to an "Executive Routine" which selects, and modifies if necessary, the appropriate input data, runs the LIRAQ model and directs the computed results to the desired output medium. Although this does isolate the user from the workings of the model it was felt necessary because of the model's very complexity and the large amounts of data which must be manipulated.

Conclusion

In conclusion, we might say that development and implementation of a complex air quality model can be reduced to a process of Communication and Compromise. The user and modeler are hopefully knowledgeable in their diverse fields. There must be a mutual understanding of the existing requirements and constraints. The modeler must make many compromises in his effort to describe the real world with the various facilities available to him. He must remain aware of the possibility that no viable compromise exists, since it would be most unfortunate to learn this only after the expense of model development. The user, for his part, must recognize the limitations which do exist and be able to operate within them. Finally, there must be interfaces which permit the user to communicate with the model in his own terms.

Acknowledgements

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A GENERIC SURVEY OF AIR QUALITY SIMULATION MODELS*

G. D. Sauter
University of California Lawrence Livermore Laboratory
Livermore, California 94550

Abstract

This survey of the generic types of models which have been developed for numerical simulation of air quality compares and contrasts them on the basis of such criteria as the simplifying assumptions made in the solution of the general continuity equation, the problems to which each model type is applicable and not applicable, the requirements for input data, and computational speed.

Introduction

A variety of generic types of numerical models for simulation of air quality have been or are being developed. The various types can be described in terms such as the assumptions on which each is based, the applications to which each is suitable and not suitable, the amount and quality of input data each requires, and the demands which each places on users (e.g., operational costs, computer capacity, expertise of operational personnel). Successful use of any air quality simulation model requires a satisfactory matching of the user's needs and resources with the model's capabilities and requirements. Therefore, in deciding whether to use air quality simulation models, and if so which ones are most suited to his needs, a potential user must not only realistically assess the goals he wishes to obtain via modeling and his resources for accomplishing them, but also understand the capabilities and requirements of the various candidate models.

This paper is devoted to a brief survey of the capabilities and requirements of the generic types of numerical air quality simulation models presently available. As a general rule, the more that one requires of a model (e.g., good spatial and temporal resolution, the ability to treat simultaneously a number of pollutants, accurate description of relevant physical and chemical processes), the greater the resources (e.g., computer capacity and cost, quality and quantity of input data) he must make available.

The Basis for Numerical Simulation of Air Quality

Numerical air quality simulation models are designed to simulate, with varying degrees of sophistication, the physical and chemical processes which govern the mixing, modifying, and transporting of atmospheric pollutants from their sources to other points of interest, often designated as receptors. The important processes which determine the variation with time of the average concentration over an arbitrary volume element of a pollutant species of interest are:

1. The net transport of the pollutant into the element by advection; i.e., due to divergence of the pollutant flux, the product of concentration and the local average wind vector.
2. The net transport out of the element due to dispersion and diffusion. These transport mechanisms result from turbulent fluctuations in the mean winds.
3. The emission of the pollutant into the element by sources within or on the lower boundary of the element.
4. Creation or destruction of the species within the element by chemical reactions between species and photochemical reactions triggered by incident solar radiation. The strength of any particular reaction is generally proportional to the product of the concentrations of the species involved. This means that for chemically reactive species, the total concentration cannot be determined by adding together the contributions from all significant sources.
5. Physical loss or destruction mechanisms such as surface deposition, decay, or rainout.

In principle, one can write a mathematical description of each of these processes and combine the various terms in a continuity (conservation of mass) equation, for each species of interest, of the form:

$$\left\{\begin{array}{l}\text{Net rate of change of}\\ \text{the average concentration}\\ \text{in an arbitrary, well-mixed}\\ \text{volume element}\end{array}\right\} = \left\{\begin{array}{l}\ \text{net rate of advection into element}\\ +\ \text{net rate of diffusion into element}\\ +\ \text{rate of source emission into element}\\ -\ \text{rate of physical loss out of element}\\ +\ \text{net rate of chemical production}\\ \qquad\text{within element}\end{array}\right.$$

The series of equations can then be solved to determine the spatially and temporally varying concentrations of all pollutants of interest. In practice, it is not possible to write down and solve the continuity equation in all generality for even a single non-reactive species; among other things diffusion and loss mechanisms are not fully understood. The situation for reactive species is even more ambiguous; not only do the chemical reaction terms couple the continuity equations for many species and make the equations non-linear, but also many of the significant reactions are poorly understood. Even if all the physical and chemical processes were well known, available meteorological and source emissions data are invariably of insufficient quality and quantity to allow an accurate simulation.

Thus in any practical numerical air quality simulation, a simplified form of the continuity equation is solved. The simplifications are generally of three types:

1. Approximation or neglect of spatial dependences
2. Approximation or neglect of temporal variations
3. Approximation or neglect of one or more of the terms in the continuity equation.

In practice, most models incorporate simplifications of all three types. For example, one can assume that all meteorological parameters and source emission rates remain constant over a time interval (say 3 hr) and then change to new but constant values over the next interval, etc. Or one might use a highly simplified set of chemical reactions in formulating the chemical production term. Depending on the simplifications involved, different air quality simulation models are applicable to different problems or situations. No single model is applicable to all problems. Although no model represents any practical problem with total accuracy, well-formulated and applied air quality simulation models can be used to gain, at reasonable levels of effort and cost, insights into air quality problems which it would not be feasible to obtain by any other means.

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*Work performed under auspices of U. S. Energy Research and Development Administration contract W-7405-Eng-48.

Highly Simplified Models

Rollback Models

Rollback models are the simplest air quality simulation models. Their real objective is the determination of the degree to which source emissions must be reduced if some desired air quality is to be obtained. In their simplest form, rollback models are based on the assumption that the local concentration of a pollutant above its background level is directly proportional to the strength of all neighboring source emissions of that pollutant. Such an assumption only applies to stable pollutants which do not undergo significant production or removal via chemical reactions. The proportional assumption applies only if the same fractional degree of control is applied to all sources. The fact that nearby sources make a larger contribution than those further away is not recognized. In non-linear rollback models, only selected emission sources are reduced, often with different fractional reductions for different sources. Some attempts have been made to use the rollback technique for ozone by applying it to oxides of nitrogen and hydrocarbons, the precursors of ozone, but the results have been inconsistent and not particularly encouraging.

In addition to their not being useful for reactive pollutants, the applicability of rollback models is limited by other factors. According to these models the spatial and temporal variations in air quality will be the same in the future as observed now. Changing spatial and temporal distributions of source emissions and meteorological patterns do not impact on air quality; source strengths are all-important. The models do have two important advantages. First, from an operational point of view, they are very easy to apply. Second, and more important, rollback models are one of the two types (Gaussian plume models are the other) which are officially sanctioned by the EPA for use in developing implementation plans for the satisfaction of ambient air quality standards.

Gaussian Plume Models

The most frequently used air quality simulation model is the semi-empirical Gaussian plume formulation. In its basic form the model assumes a time and spatially independent horizontal wind field, a time independent point source, and no chemical reactions or loss mechanisms. Turbulent diffusion in the direction of the wind is assumed negligible, and diffusion in the cross-wind and vertical directions is assumed to produce a Gaussian (bell-shaped) concentration profile about the plume centerline. The resulting downwind concentration of the plume can then be expressed in closed form as a function of the source strength, the average wind velocity, and two diffusion parameters whose values have been determined empirically for the various classes of atmospheric stability. The plume is assumed to expand indefinitely in the upward vertical direction and to be totally reflected at the surface of a flat topography. The basic plume equation is sometimes multiplied by a decay factor to simulate a simple loss mechanism.

The basic plume equation can be used to treat the case of multiple point sources by summing the pollutant concentration contributions of the individual sources. In the same way, continuous linear or area sources can be decomposed into an appropriate set of source elements and handled as multiple point sources. If the emissions are uniform over the linear or area source, a closed form, analogous to the basic point source form, can readily be developed. In any event, the size of the complex source region should be limited to one over which the meteorology can be assumed reasonably uniform. Also, the summation technique restricts the applicability of the Gaussian plume model to non-reactive species.

The major advantages of the Gaussian plume models are their simplicity and ease of application; the closed-form solutions can readily be converted to graphical, tabular, or nomogram form. This advantage is lost, however, if the model is applied to a many source, many receptor situation. Other advantages are that these models require very little input data and that there is considerable experience in their use.

The major limitation in the applicability of plume models is the assumption that the wind field is constant and uniform. In practice this limits their use to time periods on the order of an hour and spatial distances on the order of 10 km. Quasi-steady-state applications can be made by periodically updating the source emissions and meteorology, but this does not alleviate the spatial limitation. Further, since the predicted pollutant concentration is inversely proportional to the wind speed, the model is not applicable on calm or nearly calm days. Finally, the model is not applicable in situations with complex topography or low altitude inversions.

Gaussian Puff Models

The Gaussian puff model was developed to overcome some of the limitations of the plume equation, particularly the time independence. In its basic form, the model tracks a puff of pollutant emitted from a point source as it is blown downwind and diffused in a Gaussian manner. The puff is allowed to expand in volume so that all of the original pollutant mass is retained within it. In the quasi-time dependent case, the wind field and source emission rate are periodically updated and assumed constant over each time interval. In the steady-state limit, the puff model is equivalent to the plume model. As with the plume model, multiple source situations are treated by summation, with due consideration taken of the time for puffs from the various source elements to reach the receptor. The cross-axis distribution within the puff need not be assumed to be Gaussian; in one refinement, cross-axis diffusion is determined from turbulent eddy diffusion (k) theory.

Although it does permit some degree of time dependence, the puff model suffers from some of the other limitations of the plume model; i.e., only non-reactive pollutants can be treated for cases of relatively flat topography (some rather unsuccessful attempts have been made to incorporate a simplified treatment of reactive species). It can be used in light wind situations. The time dependent puff model is not as easy to apply as the plume model. Time dependent source data are required, and time dependent trajectories must be determined. These more difficult operational problems tend to outweigh the added advantages of the puff model, and it is not widely used. It is best applied to cases of a few sources and a few nearby receptors. Even here a computer is generally required. For widely distributed sources and multiple receptors, the large number of trajectories required makes the use of the puff model prohibitive.

One Box Models

These models are based on the assumption that pollutants are uniformly mixed throughout a fixed volume (box) of air. For air quality simulation (as opposed to simulation of smog chambers), the box is usually taken to extend vertically from the terrain surface to the inversion base; horizontally the box should cover an entire region of distributed sources. In the simplest applications no transport of pollutants into or out of the box is allowed. The resulting concentrations are then proportional to the total rates of source emissions of pollutants into the box and inversely proportional to the average residence time and the inversion base height. Since pollutant clouds must generally travel distances on the order of 5-10 km before uniform mixing can occur, simple box models should only be used to estimate average concentrations over large area sources (e.g., whole cities) or to simulate background concentrations at points with no large local sources nearby.

Models which are essentially a special type of box model have been developed by Gifford and Hanna at NOAA's Atmospheric Turbulence and Diffusion Laboratory. For non-reactive pollutants, the simple ATDL dispersion model can be expressed as $c = A\,Q/u$, where c is the average pollutant concentration in the box, Q is the average source emission rate per unit area, and u is the mean wind speed. The dimensionless parameter A is assumed to be a constant for a given atmospheric stability; analyses of air quality data for a number of urban areas suggest that, over long averaging times (month, season, year), $A = 225$ is a reasonable value. The ATDL dispersion model is a reasonable one to use in determining average concentrations of non-reacting pollutants over large areas and long averaging times. If the area considered is too small, the effects of sources outside the region under study may be significant; if the averaging time is too short, the model will not effectively account for significant short-term deviations from average source emission rates and meteorology. Operationally, the ATDL model is very easy to apply, and it requires a minimum of input data. Its major drawback is the lack of spatial resolution over large areas.

Hanna has also applied the ATDL model to several reactive pollutants by incorporating a very simplified set of chemical reactions. For example, all reactive hydrocarbons are lumped together as a single species. The resulting model has five parameters (instead of just one for the non-reactive model) which can be adjusted to give the best results for a particular situation. The chemical mechanism is not general; a different mix of sources and/or significantly different meteorology would necessitate a retuning of the model. As with the non-reactive version, this model is designed to determine average concentrations over a large area under typical meteorological conditions.

More Complex Models

The models described above stress ease of application at the expense of physical and chemical fidelity. They are either analytic or require very limited numerical computer capabilities, and the input data requirements are modest. (An exception is the use of the puff model with a large number of trajectories.) However their applicability is limited; e.g., simulation of a steady-state or quasi-steady-state point source (Gaussian plume model) or air quality averaged over a large area (ATDL). The models described below are designed to yield air quality simulations which include both spatial and temporal dependences. As a result, their operation is considerably more demanding, requiring extensive computer capability and quite large amounts of spatially and temporally resolved meteorological and source emissions data.

Eulerian Grid Multibox Models

An Eulerian multibox model consists of a number of constant size volume elements in a fixed spatial grid which covers the entire region of interest. Pollutants are allowed to flow through the boundaries of each element as a result of advection, diffusion, sources, and sinks. Within each element, the pollutants are assumed to be mixed; they may be chemically reactive. Time dependence is introduced by periodically (typically every hour) updating the source emission rates and the prevailing meteorology (wind speed and direction, inversion base height, and for reactive pollutants, incident sunlight) for each grid element. Thus the multibox simulations produce time histories of (hourly) average pollutant concentrations with spatial resolutions determined by the size of the grid elements. The minimum size of the elements is limited by one or both of two factors: the quality of the available source emission and meteorological input data and the memory capacity of the computer to be used. For a given computer, the minimum grid element size is determined by a combination of factors: the size of the region to be simulated, the number of pollutant species considered, the number of vertical layers of elements, the degree of sophistication of the numerical technique used, and the complexity of the chemical reaction set (if any). Increasing one or more of these factors increases the minimum grid size. Typically, the horizontal dimensions of a grid element are a few kilometers. A significant data gathering and preprocessing effort is necessary to produce realistic source emission and meteorological input data with this resolution, particularly in regions with complex topography, which tends to make both the meteorology and the source distribution less uniform.

The usual approach in calculating the flow of pollutants across the boundary of an Eulerian grid element is to use a technique based on the finite difference between the pollutant concentrations on either side of the boundary. The assumption that each element is well-mixed gives rise to errors, referred to as numerical diffusion, in the simulation of pollutant transport. These errors can be controlled reasonably well, at the expense of additional computational complexity, with higher order differencing schemes, especially for distributed rather than localized sources. Two of the most prominent examples of such models are the Systems Applications, Inc. (SAI) and Livermore Regional Air Quality (LIRAQ) models.

The SAI model, originally developed for the Los Angeles basin, uses a grid with several vertical layers, thus simulating the solution of the continuity equation in three dimensions, and in turn requiring sufficient meteorological data to adequately represent a three-dimensional wind field. The model contains a reaction set of 16 reactions covering 13 species (all hydrocarbons lumped together) which probably should be tuned for each area of application. A more extensive chemical reaction set is now being incorporated into the model.

The LIRAQ model, originally developed for application to the San Francisco Bay Area, uses a single layer of grid elements between the terrain surface and the base of the inversion layer. Only horizontal pollutant transport is simulated; within each element, the vertical pollutant distribution is represented in terms of a simplified profile. Two versions of the model exist. The non-reactive version (LIRAQ-1), when used on a CDC-7600 computer, can treat up to four species simultaneously on a 45 by 50 element grid, more than adequate to treat the entire Bay Area with 5 km resolution or subregions with finer resolution. About 15 min. of computer time are required for a 24 hr simulation. LIRAQ-2, for reactive species, incorporates a set of 48 reactions to treat 19 species, including three hydrocarbon classes. This limits a CDC-7600 simulation to a maximum of 20 by 20 elements, still enough to cover most of the Bay Area with 5 km resolution. A 24 hr simulation requires about 60 min. of computer time.

These Eulerian grid multibox models represent the most comprehensive approach to simulating air quality on a regional basis; they are applicable to such air quality problems as regional compliance with air quality standards and evaluation of the impact on regional air quality of various land use alternatives. However, because all emissions within a grid element are lumped together, these models should not be used to simulate the effect of a strong local source on nearby (within a few grid elements) receptors. Substantial input data and computer capability are required to operate these complex models, and applications are limited to simulations of a few days for "typical" or "worst case" conditions.

Particle-in-Cell (PIC) Models

These time dependent models combine the use of an Eulerian grid and marker particles, each marker representing a fixed mass of pollutant. The markers are introduced into the grid where emissions occur and are tracked as they are transported and dispersed throughout the three-dimensional grid by the specified wind field. At the end of any time interval, the concentration of a pollutant in any grid element can be determined by summing the masses represented by the particles then in the element. This technique virtually eliminates transport errors due to numerical diffusion.

The limitation on the PIC technique is the large number of particles which must be tracked to adequately represent pollutant concentrations and concentration gradients over a large grid. Available computer memory sizes limit a simulation to a combination of about 10^4 particles and 10^4 grid elements (about 30 min of CDC-7600 computer time would be required for an 8 hr simulation). This makes it extremely difficult to represent large gradients and small changes in concentrations of several species with sufficient accuracy to adequately characterize chemical reactions, so the PIC technique is best applied to non-reactive species. PIC models are perhaps the best choice for accurate three-dimensional simulations of the pollutant concentrations produced by localized sources of non-reactive species. The major effort in applying the PIC technique to urban air quality simulation has been the application of the NEXUS model by Sklarew to CO and ozone in Los Angeles.

Lagrangian Box Models

In contrast to Eulerian box models, which simulate the time history of pollutant concentrations within a volume element fixed in space, Lagrangian box models (sometimes called trajectory models) simulate the time history of pollutant concentrations within boxlike elements of constant volume as they flow along wind streamlines. A box may have one or several layers (cells) between the terrain surface and the base of the inversion height. As the box flows across a source, pollutants may flow in through the bottom of the box and diffuse vertically into other cells (if any), but usually no horizontal transport of pollutants across the boundary of the box is allowed, so numerical diffusion problems are eliminated. Within each cell the air is assumed to be well-mixed, and chemical reactions can occur. The horizontal dimensions of the box, typically on the order of a few kilometers, determine the spatial resolution of the calculated concentrations and of the required input data. Both source emissions and meteorology can be time dependent. As with Eulerian multibox models, they are usually updated on an hourly or few hourly basis.

Lagrangian box models are primarily source-receptor oriented; that is, they relate the pollutant concentration at a receptor area to specific upwind emission sources via one or more wind trajectories. Thus the user can identify the source areas responsible for observed pollutant concentrations at selected points along specific trajectories. Air quality simulations on a regional basis can be treated by tracking boxes along enough different trajectories to adequately represent the sources and meteorology of the region and interpolating between calculated trajectories. This procedure works best in areas with relatively uniform source distributions and meteorology, where the number of trajectories needed to characterize the region is reasonably small. For regions with complex meteorology and/or source distributions, the number of trajectories needed may make the computer requirements prohibitive. The ratio of time simulated to computer time required is on the order of 500 to 1 for each trajectory considered (e.g., about 30 min of computer time would be required to follow 25 trajectories over a 10 hr period). Thus, as is the case for Eulerian multibox models, simulations are limited to a day or so for typical or worst-case conditions.

Representative of Lagrangian box models is the DIFKIN model, developed at General Research Corporation, which has been applied to both the Los Angeles and San Francisco Bay regions. The model uses five vertical layers and vertical diffusivity rates that depend on atmospheric stability. The simplified chemical reaction set employs 16 reactions encompassing 13 species, with all hydrocarbons lumped together. Other models may combine more sophisticated chemistry and simpler meteorological treatments.

Conclusion

Although it has of necessity been very brief, this generic survey of numerical air quality simulation models should be sufficient to show that a variety of these models is now available. These models differ widely in the level with which they treat the important physical and chemical processes involved, in the applications for which they are designed, and in the input data and computational capacity they require. No single model is adequate for all types of air quality simulations. In selecting an air quality simulation model, a potential user should seek a good match of his resources and modeling needs with the capabilities and resource requirements of the model.

Selected References

The references listed here by no means comprise an exhaustive list. Rather, they have been selected to be representative of the air quality simulation models currently in use. The references generally contain further references to generically similar models.

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AIR QUALITY MODELING - A USER'S VIEWPOINT

Richard H. Thuillier

Chief of Research and Planning
Bay Area Air Pollution Control District, San Francisco, California

Summary

A requirement for modeling has developed out of the Clean Air Act amendments of 1970. In spite of this requirement and the existence of a variety of modeling techniques, there is a prevailing reluctance toward the use of modeling as a decisionmaking tool. Based on experience with regional application of a variety of models, the Bay Area Air Pollution Control District encourages the use of appropriate techniques in a coordinated regional context. The District feels that much can be gained from simplified approaches at minimal cost and recommends that regional resources be pooled for effective, efficient, and standardized application.

Introduction

The Bay Area Air Pollution Control District (BAAPCD) has regulated air pollutant emissions in the nine-county San Francisco Bay Area over a period of 20 years. Traditionally, such regulation has been accomplished, by and large, through best effort technological control of point sources, with air quality improvement as a general goal. Control program effectiveness has been measured against the yardstick of air monitoring data from community-representative sites.

With the advent of the Clean Air Act amendments of 1970 and ensuing Federal regulations, there developed a requirement for a more structured approach to air quality control. The promulgation of ambient air quality standards and associated compliance schedules has given rise to a concept of air quality control and analysis based on more precise relationships between source emissions and their resulting air quality impact. The activities involved in establishing such relationships and using them effectively in an air quality control context comprise the challenging field of air quality modeling.

Notwithstanding the existing requirement for modeling, relatively little has been done in exploiting the potential of this emerging technology. The evident reluctance to use modeling is engendered by such factors as esoteric techniques, required resources for model use, and a general confusion regarding appropriate application.

Immediately after the promulgation of the Clean Air Act amendments, the BAAPCD made an extensive commitment to modeling in all its facets. In a region as extensive as the Bay Area, air quality standards can be achieved only if planning decisions properly consider air quality. We feel that modeling can provide appropriate air quality input to decisionmaking and is, therefore, a very useful tool for planning and regulating air quality. We are grateful for this opportunity to discuss our philosophy and experience in this regard, with a view toward stimulating greater interest within the user community.

Institutional Framework for Modeling Application

In attempting to fulfill the requirements of the Clean Air Act, control measures must be conceived and applied on a coordinated, regionwide basis with consideration of all sources of pollution in terms of their combined impact upon receptors. A control program of such scope cannot proceed effectively toward desired levels of air quality without the unifying guidance of a regional air quality model. Throughout this presentation, the term "model" should be construed to refer not to a single algorithm or computer code but rather to an integrated and compatible set of analytical tools which, together, supply the necessary quantitative relationship between regionwide sources and receptors in the context of defined air quality standards.

One of the principal problems associated with modeling in a regional context arises from a broad spectrum of source categories and a variety of jurisdictional responsibilities. Incompatible data bases, divergent institutional resources, and special interest bias can serve to place air quality control more in the context of an adversary proceeding than in the context of a coordinated technical effort. Since such controversy has a tendency to divert energies and obscure goals, the interest of air quality attainment and maintenance can best be served by resolution of such conflicts. In this regard, two possible approaches suggest themselves: One approach would be the vesting of all responsibility for air quality analysis in a single agency with regionwide jurisdiction. An alternative approach would be to continue with a decentralized analysis responsibility under a unified code of procedures involving, for effectiveness, an integrated, complementary use of diversified resources and compatible techniques. The latter appeals to the author from the standpoint of political acceptability as well as technical feasibility. Ideally, such an approach would proceed under the guidance of a highly qualified multidisciplinary technical committee, group, or team, with sole responsibility for the development, dissemination, and coordination of standardized procedures for the region. Such a team could also be responsible for interpretation of modeling results.

In the Bay Area, a combination of the two approaches prevails. In 1972, the BAAPCD created a multidisciplinary Research and Planning Section within the District's Technical Services Division with responsibility for air quality model development and application. Over a 3-year period, the group has developed a sizeable inventory of techniques. As an agency with regional jurisdiction and in view of its experience with air quality models, the District has been able to exercise regional leadership in air quality modeling activity. We have, however, been greatly assisted in our efforts by other regional agencies possessing specialized resources and expertise not available in-house. The District, in turn, provides guidance and assistance to a variety of agencies and individuals who wish to do their own analysis in a way which is mutually acceptable to the analyst and the District. Current efforts in air quality maintenance planning should serve to further the interest of a coordinated institutional effort in the regional solution of air quality problems.

The Relationship of Modeling to Decisionmaking

In addition to technical and institutional problems as discussed above, another barrier to the effective use of modeling technology is a confusion or misunderstanding of the relationship of modeling to the decisionmaking process. It is important to realize that decisionmaking is inherently subjective. The concept of a decision implies a choice among alternatives involving an element of uncertainty. Decisionmakers deal with the reality of uncertainty and their decisions are conditioned by but not necessarily dependent upon the amount or quality of available information.

These factors are frequently overlooked when modeling is proposed as an air quality analysis tool. One of two alternative, contradictory, and equally unwarranted arguments will frequently be lodged against the adoption of a modeling program. On the one hand, it is argued that the uncertainties in the models will render them useless as input to the decisionmaking process. On the other hand, it is argued that the valued judgment of the decisionmaker will be replaced by the model itself as an objective but utterly inscrutable and possibly flawed arbiter. With regard to these arguments, we note that mandated decisions relating to air quality must be made on the basis of available information. Modeling results may or may not influence a decision but as added information cannot conceivably detract from the quality of that decision. The alternative to consideration of modeling information, whatever the degree of uncertainty, is all too often a complete disregard of the air quality issue. In our experience, the contribution of modeling is a positive one, serving to clarify the decisionmaking process and to make decisions less arbitrary in nature. With regard to the installation of a model as an objective arbiter, we feel this is rather unlikely in view of the very imperfections used as a basis for the first argument. In reality, modeling output must invariably be subject to interpretation before a decision can be based in any way upon it. In the interest of efficiency, however, standardization of routine procedures and the development of criteria based on accepted modeling techniques may be desirable.

In summary, modeling results should be viewed as nothing more than information input to the primarily judgmental process of decisionmaking. Such information may be weighed with other factors in arriving at the decision. Modeling uncertainties, whatever their nature or extent, should be considered simply as part of the general store of uncertainty inherent in the decisionmaking process. If this viewpoint is taken, then there is nothing to fear from modeling except, of course, fear itself. Within a carefully structured, institutionally integrated and professionally administered program, we feel that modeling can be a very effective decisionmaking tool.

Model Selection and Application

To be most effective, models should be selected to complement available resources and flexibly address the problem area in which they will be applied. Applications in the Bay Area run the gamut from regional planning to project review. To meet our needs, we have adopted the modular system outlined schematically in Figure 1. Modeling is done on three spatial scales of

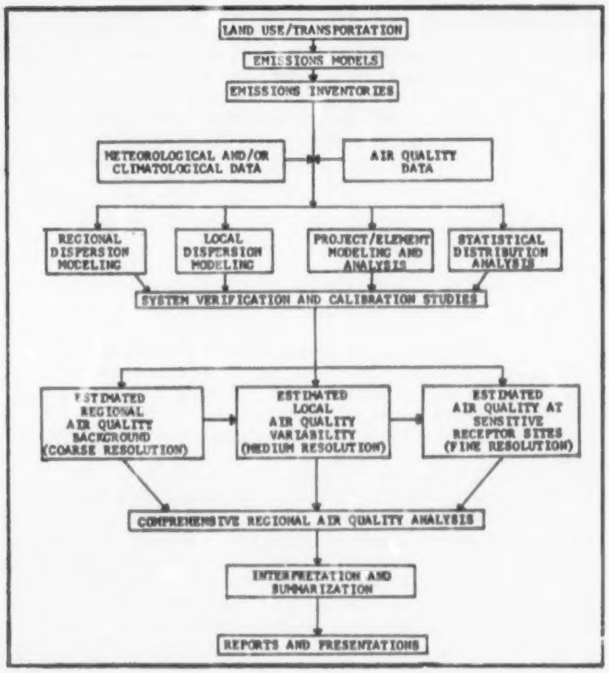
LAND USE/TRANSPORTATION
EMISSIONS MODELS
EMISSIONS INVENTORIES
METEOROLOGICAL AND/OR CLIMATOLOGICAL DATA
AIR QUALITY DATA
REGIONAL DISPERSION MODELING
LOCAL DISPERSION MODELING
PROJECT/ELEMENT MODELING AND ANALYSIS
STATISTICAL DISTRIBUTION ANALYSIS
SYSTEM VERIFICATION AND CALIBRATION STUDIES
ESTIMATED REGIONAL AIR QUALITY BACKGROUND (COARSE RESOLUTION)
ESTIMATED LOCAL AIR QUALITY VARIABILITY (MEDIUM RESOLUTION)
ESTIMATED AIR QUALITY AT SENSITIVE RECEPTOR SITES (FINE RESOLUTION)
COMPREHENSIVE REGIONAL AIR QUALITY ANALYSIS
INTERPRETATION AND SUMMARIZATION
REPORTS AND PRESENTATIONS

Figure 1a. Flow Chart of Regional Air Quality Modeling Activity in the San Francisco Bay Area.

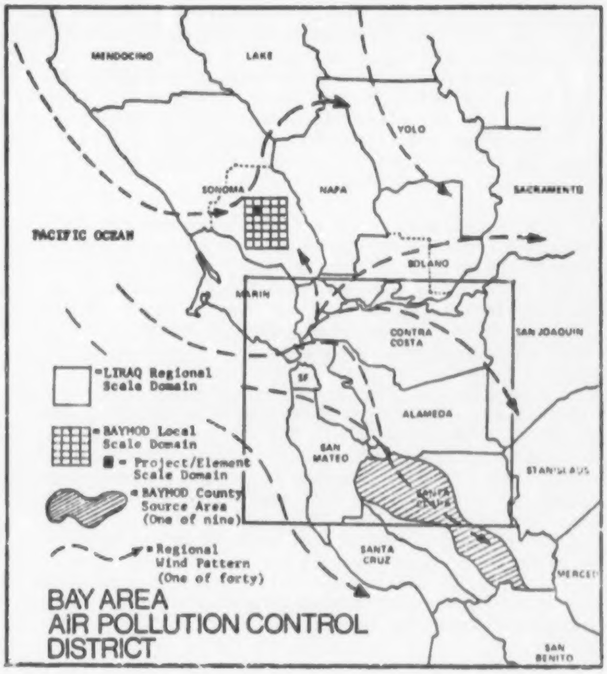
MENDOCINO
LAKE
YOLO
SONOMA
NAPA
SACRAMENTO
PACIFIC OCEAN
SOLANO
MARIN
CONTRA COSTA
SAN JOAQUIN
SF
= LIRAQ Regional Scale Domain
= BAYMOD Local Scale Domain
= Project/Element Scale Domain
= BAYMOD County Source Area (One of nine)
= Regional Wind Pattern (One of forty)
ALAMEDA
SAN MATEO
SANTA CLARA
STANISLAUS
SANTA CRUZ
MERCED
SAN BENITO
BAY AREA AIR POLLUTION CONTROL DISTRICT

Figure 1b. Setting for Regional Air Quality Modeling Application in the San Francisco Bay Area.

resolution using techniques of the simplest type consistent with physical setting and application requirements of the scale in question. A statistical model supplements and links the temporal resolutions of the various modeling techniques. Meteorological, climatological, and source emissions data bases are available in various formats as input to the modeling. The system is designed to provide air quality estimates at three spatial scales, independently, in a manner that enables successively coarser scales to be treated as background. The statistical model enables us to address the air quality problem directly in terms of the ambient air quality standards over appropriate averaging times.

The modular, multifaceted nature of our system allows us to deal effectively with a variety of applications at appropriate levels of time and cost with our own in-house resources or in collaboration with outside agencies or individuals. We feel that existing techniques, judiciously employed, enable us to provide useful input to decisionmaking in virtually all of our air quality problem areas.

Figure 2 illustrates photochemical modeling output within the regional scale domain in Figure 1. The model LIRAQ-2[1] estimates concentrations of ozone, nitrogen oxides, hydrocarbons, and carbon monoxide at a regional resolution of 25 km^2. Finer resolutions of 4 km^2 and 1 km^2 are available for subregional analysis and a less complex version of the model, LIRAQ-1, is available for nonreactive analysis alone. The model accounts for the perturbed airflow through complex terrain providing a field of concentrations hour by hour or a time history at selected points based on emissions and meteorological data input chronologically. The principal use of this model will be in the evaluation of regionwide planning or regulatory alternatives. The frequency of model application, using a CDC 7600 computer, is somewhat limited by cost.

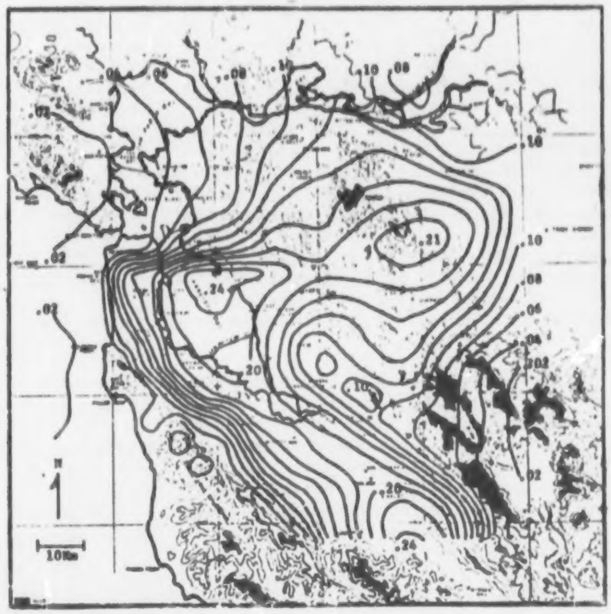

Figure 2. Estimated Distribution of Ozone Concentrations at 1400 PST, 26 July 1973 by LIRAQ-2 Regional Photochemical Model. Concentration Units Are Parts Per Million With an Isopleth Spacing of 0.02 PPM.

For the purpose of local scale analysis, the District has developed a gaussian model, BAYMOD.[2] This model provides annual average concentration estimates for nonreactive pollutants over a 690 km^2 local area at a resolution of 1 km^2. Annual average emissions and wind speed data are input as a 690 element (30x23) grid of 1 km squares. A local wind rose is utilized for annual weighted average transport from upwind grid squares treated as point sources. Concentrations from sources within the same grid square are calculated as an integrated line source average. The model may be made to treat local sources alone or to include county-scale regional background through use of a box model in conjunction with transport by regional wind patterns. Larsen's statistical model is used in conjunction with historical monitoring data to relate annual averages to averaging times associated with air quality standards.[3] BAYMOD is run routinely on the District's in-house Hewlett-Packard 3000 minicomputer. Typical applications are air quality analysis of local plan alternatives and the estimation of pollutant background concentration for use with more localized analyses. Individual local analyses may be assembled in mosaic form to provide larger regional coverage at fine (1 km^2) resolution. Figure 3 is sample output from BAYMOD in the vicinity of the city of Santa Rosa, within the local scale domain in Figure 1.

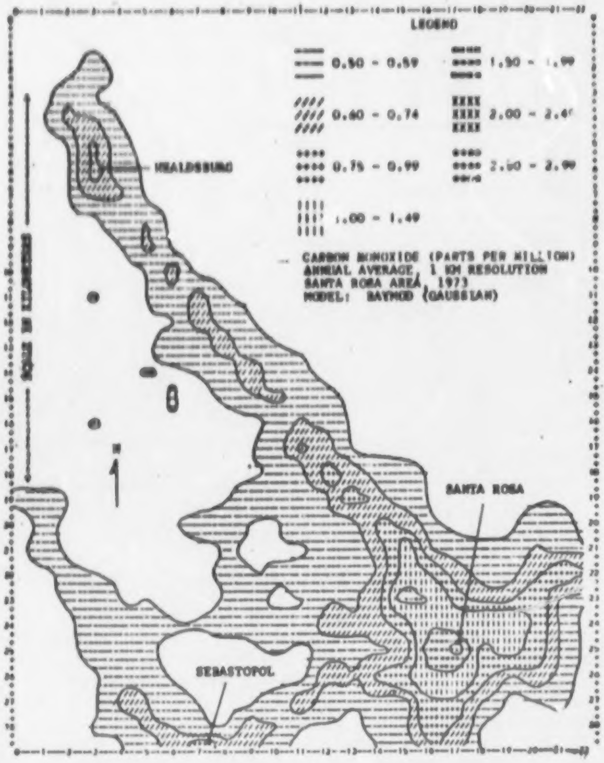

Figure 3. Estimated Distribution of Carbon Monoxide Concentration (Annual Average) in the Vicinity of Santa Rosa, California, by the BAYMOD Regional Gaussian Model.

The final module in the District system is at the project/element scale. Standard gaussian, single and multiple point, and line source techniques are employed to estimate the air quality impact of stacks, roads, housing developments, shopping centers, airports, and a variety of other projects and project source elements, as illustrated by Figure 4. Principal applications are for permit review, variance hearings, and the review of environmental impact reports. Modeling is done using either computerized codes developed in-house or by manual or nomographic methods, depending on the scope and time frame of the analysis. To fill a large number of requests for assistance in project-level air quality analyses by non-District individuals and agencies, the District has prepared a comprehensive set of guidelines involving manual techniques in "cookbook" format.[4] The popularity of this publication is indicative of an existing need for user assistance.

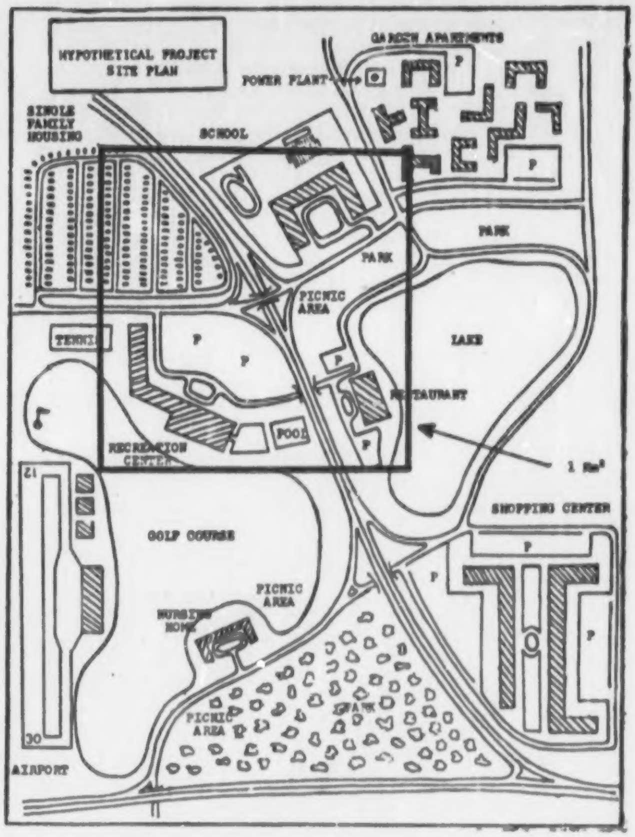

Figure 4. Illustration of a Typical Setting for Modeling Application on the Project/Element Scale.

Simplifications, Assumptions, and Parameterizations

Perhaps one of the greatest drawbacks to effective model application is the esoteric nature of many techniques. There is an allure associated with sophistication perpetuated by the aesthetic appeal of complex technology and by an intuitive feeling that complex problems can be solved only by complex methods. As a general rule, we feel that sophistication should be sought only when there is true complexity in the nature of the problem solution and when the quality of the input data is commensurate with the requirements of the model. The photochemical process will normally require modeling complexity while nonreactive modeling is amenable to considerable simplification. The principal benefit to simplicity, aside from cost, is the increased breadth of application through frequent and multiple use. If the outputs of various models are compared in the context of the information required, the merits of simplification may be readily assessed.

Frequently, the modeling process can be simplified through proper definition of the problem and appropriate parameterization of the modeling scheme. For example, in assessing carbon monoxide levels in a local area, we might initially consider a model which would provide point values of concentration at multiple locations and at discrete time intervals. With such a model we could then evaluate the highest point concentration in the area during the period of peak traffic flow under the most adverse meteorological conditions. If, however, we determined that point values were not of interest in our study area due to spatial mobility of receptors (people), more appropriate spatial averages might be obtained by a far simpler and less costly approach.

An argument against the application of simplified techniques in air quality regulatory situations is based on the premise that the social and economic consequences of such decisions are too important to be based upon analyses exhibiting less than state-of-the-art accuracy and precision. While the premise is undoubtedly correct, care must be taken to avoid a never-ending search for the perfect model. Simplification is consistent with the premise if "state-of-the-art" is defined to include considerations of data base condition, problem definition, and required information, in addition to the conceptual and algorithmic structure of the analysis scheme itself. When the choice of model includes such considerations, useful estimates can frequently be made with available techniques at minimal cost. The District makes liberal use of such techniques and recommends them to others for a wide range of applications. Our efforts in this regard have resulted, we feel, in a greatly increased willingness to include air quality considerations among the many factors normally involved in land use and other decisions.

Monitoring, Modeling, and Regulatory Relationships

Historically, disparate motivations have influenced the formulation of air quality regulations, the setting of air quality standards, the establishment of air monitoring programs, and the development of air quality models. Regulations have normally been source-oriented, focusing on equipment or performance characteristics with a view toward ease of enforcement. Air quality standards are receptor-oriented focusing on time-averaged ambient concentrations relatable to effects on health or welfare. Air monitoring has been site-oriented with a view toward representative sampling under economic and facility constraints, and finally, model development has been guided by computations technology under data constraints.

In complying with the comprehensive requirements of Clean Air Act legislation, efforts in modeling, monitoring, and regulation should ideally be integrated in a compatible and complementary systems approach to air quality analysis. While complete compatibility may never be achieved, many improvements are possible over the present conditions. In the interest of such improvements, we offer the following comments:

1. Spatial averaging should be incorporated wherever possible in the definition and interpretation of air quality standards as well as monitoring

programs. Thus, for example, the standard for pollutant X might be defined as Y parts per million as a spatial average over Z square kilometers. Similarly, air monitoring using statistical/mobile techniques might provide estimates of existing air quality as a spatial average on the same scale. An appropriate spatial definition would accommodate the resolution limitations of modeling input as well as the spatial mobility of human receptors over the averaging times inherent in the dosage-oriented air quality standards. In addition, modeling output could be compared, for validation, with air monitoring data on a compatible spatial scale.

2. Modeling should be incorporated in source performance regulations to achieve consistency between emission limitation and desired air quality. Thus, a regulation might limit source emissions to a rate which, on the basis of a given dispersion algorithm, would maintain ground-level concentrations at a specified level.

3. Air monitoring should be performed at places other than the traditional downtown urban locations to better define regional gradients. Data from nonurban sites would facilitate the validation of modeling techniques and would provide needed information on background levels of pollutants from natural sources.

Conclusions and Recommendations

Our experience has convinced us that air quality modeling is a very useful tool for air quality regulation and planning. Specifically, modeling has given us a consistent rationale for decisionmaking and enabled us to provide technically-supportable solutions to a great variety of problems. We feel that under the guidance of appropriate expertise and with sufficient ingenuity, very simple techniques can be applied effectively at minimal cost. We realize that air quality problems and appropriate modeling techniques often substantially differ from region to region, and for that reason, no single technique or set of techniques can be applied universally, with success. We feel, however, that the store of existing techniques is flexible enough to provide useful solutions to air quality problems in almost any set of circumstances. Finally, we feel that, notwithstanding the demonstrable limitations of modeling technology, decisions based on modeling results, professionally interpreted, will better serve the interests of air quality than those based on intuition alone.

We highly recommend that the framework for a comprehensive and standardized program of model application be established in each region with existing or potential air quality problems. A small interdisciplinary staff dedicated to the task of regional modeling can provide appropriate guidance for the solution of air quality problems and the efficient utilization of resources. In the interest of establishing such regional capabilities, we would suggest that consideration be given to state and Federal encouragement as well as funding. Our own experience in this regard has been very positive, and we have welcomed the opportunity of sharing our feelings and ideas at this conference.

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SPACE: A CLOSER LOOK AT THE IMPACT OF ENVIRONMENTAL POLICY

Ernest Heilberg
Chase, Rosen & Wallace, Inc.,
Alexandria, Virginia

Abstract

The Spatial Pollution Analysis & Comparative Evaluation (SPACE) System is a computer-based model system designed to indicate the impact of local policy decisions on the environmental quality within metropolitan areas. This system was developed as an adjunct to the Strategic Environmental Analysis System (SEAS) and relies heavily on data produced by SEAS.

Major features of SPACE include:

1. The determination of net emissions and ambient levels of pollution resolved to a grid system covering the analyzed region.

2. The ability to introduce a broad variety of local environment-related policy changes.

Introduction

Contrary to what the acronym may at first suggest, the SPACE System deals with matters very close at hand - pollution within metropolitan areas. The actual name, The Spatial Pollution Analysis and Comparative Evaluation System, was intended to point out that the system is concerned with the spatial distribution of pollution, rather than just cumulative or average values for the region considered. This is the concept of "space" you should associate with this system.

There are several important aspects of the SPACE System which are not indicated by the name. First, as suggested before, the "space" in question is that within a metropolitan area, specifically an SMSA (Standard Metropolitan Statistical Area). Second, the system has been designed to be sensitive to a broad range of local environment-related policies. Finally, the system has been developed as an extention of SEAS (the Strategic Environmental Assessment System).[1] All of these features will be discussed in more detail later.

Putting these features together, the intended applications of SPACE should begin to become apparent. The SPACE model system is essentially a planning tool, for use by both national and local planners, in screening environment-related policy options. Three specific categories of application were considered during the system design efforts:

1) Use by local planners to compare the relative effectiveness and efficiency of local environmental quality improvement plans.

2) Use by EPA planners (in conjunction with SEAS) to determine the impact of national policies on metropolitan areas.

3) Use by EPA planners, in their development of guidelines for local planners, to compare the effects of specific local policies on various types of metropolitan areas.

To provide for these applications, SPACE was designed to consider a broad range of policies as well as a variety of impacts of such policies. As a result, SPACE can be used as a policy screening tool with applications far beyond those initially intended, e.g. inclusion of an energy submodel would permit studies involving both pollution and energy policies. Some of the other possible applications will be alluded to later.

Background

Before proceeding with the discussion of SPACE, it will be useful to review SEAS, especially those elements of SEAS which are most pertinent to SPACE. SEAS is a large, complex collection of forecasting models which relate the national economy to the generation of pollution residuals and the associated costs of pollution control. It provides a framework within which a decision-maker can assess the impact of alternative national policies related to the economy and the environment.

SEAS is driven by a Leontief-type economic (input-output) model which forecasts the expected levels of the various economic sectors in the U.S. over a 15 year period. These projections are converted to pollution forecasts, by considering the technologies involved for operation, production and abatement. The economic and pollution forecasts are then disaggregated to various sub-regions of the nation, e.g. states, SMSA's, etc., by considering the relative characteristics of the subregions. To insure completeness, pollution sources not directly related to the economic sectors (e.g. related to households and transportation) are introduced at the disaggregated levels and aggregated upwards.

Using SEAS it is thus possible to estimate the amount of the various pollution residuals that can be expected to be generated nationwide or within specified sub-regions of the nation, and to note the possible changes in these estimates that result from implementing various national policies. It should be obvious that the results obtained are most meaningful when considering the nation as a whole or the larger subregions. As consideration turns to the smaller sub-regions, e.g. SMSA's, local policy decisions can be expected to have a significant impact not reflected in the SEAS analysis.

The desire to provide for the more meaningful use of the disaggregated projections led to the conception of the SPACE System. To demonstrate the feasibility of this concept, the Washington Environmental Research Center of EPA let a contract to Chase, Rosen & Wallace, Inc. (CRW) and Alan M. Voorhees & Assoc., Inc. (AMV) to develop the SPACE Test System. It is this test system, completed in mid-1975, that is the subject of this presentation.

SPACE System Applications

SPACE is a working system which can be of value in problem solving. Its main utility is as a tool in comparing the relative impact of various local policy options on pollution in a metropolitan area. Thus, for a locality attempting to meet specific environmental goals, SPACE could be useful in screening policy alternatives.

The policy alternatives that can be treated are essentially unconstrained by the SPACE System. These include: (1) direct pollution control programs, such as improving the capacity and/or quality of solid waste management systems or water treatment systems, setting stricter emission standards for factories or motor vehicles; (2) land use controls, such as zoning, limiting emissions in specific locations, designating open land, selecting specific sites for major facilities (e.g. airport, sports arena, etc.); (3) auto use deterrents, such as establishing auto free zones, designating special bus and car pool lanes, improving mass transit, increasing fuel and parking costs; and (4) other indirect means, such as providing economic incentives for private emission control actions, establishing constraints on use of specific fuel types. This listing is by no means exhaustive; but rather, illustrates the broad range of possible considerations.

The metropolitan areas that can be considered are limited only by the availability of data. As will be discussed later, EPA has taken steps that should ultimately eliminate this limitation. With data available for sufficient SMSA's, it will be possible for EPA to determine the differing impact of specific policies on different types of cities. Guidance provided by EPA to local planners could thus be tailored to the specific locality.

By design, SPACE measures the impact of policy options in terms of pollution. In the process of making such determinations, the system becomes involved in analyses related to local economic activity, land use, transportation, and energy. With minor modifications, mainly related to the massaging and display of intermediate results, the possible applications of SPACE can be extended to include the measurement of policy impact in a variety of forms. For example, SPACE could indicate the trade-off between pollution generated and fuel consumed resulting from policies that encourage or discourage use of specific fuels; or it could indicate the inability of the region to meet the SEAS economic projections as a result of policies constraining factory emissions. The combination of the wide range of policies that can be treated and the variety of impact measures possible, results in a highly flexible model for local policy screening.

SPACE System Overview

The metropolitan area under study is initially a flat, relatively empty rectangular grid system. It contains rivers, highways, railroad tracks, but little else. For each analysis year the SEAS projections indicate the amount of residential, industrial, commercial, and other developments that are expected to exist in the region. These are distributed over the grid system by considering the attractions and constraints associated with individual grid squares, the features of neighboring grid squares, and the historical land use patterns. This distribution is intended to be representative, not predictive. Each activity thus located becomes a single stationary pollution source.

In addition to any pollution generated directly by these activities, each activity has the potential of attracting pollution through the motor vehicles that come to or leave its facilities. These mobile pollution sources are given location in the grid system by associating trip ends directly with the located activities and by distributing the trip routes over the implied transportation network.

With both stationary and mobile pollution sources located, gross pollution generated in each grid square is determined, based on size and type of each source. The actual pollution emitted to the environment is next determined by considering two types of pollution modification - transformation and transportation.

Pollution transformation generally involves some technological process for converting the polluting substances into other substances. These other substances may also be considered pollution, as in the case of burning solid waste to produce a smaller volume of ash plus air pollution. Some of the new substances may, however, be useful materials, as in the conversion of some solid waste to fertilizer.

Pollution transportation refers to the physical movement of the residuals from one location to another, generally with no significant change in the substances transported. This includes the piping of sewage waste to treatment plants and the hauling of solid waste to land fills and incinerators. At their destination this transported pollution may be transformed.

The transportation of pollution residuals to activities which may in turn transform them introduces a special concept. Each category of activity is designated as being either "exogenous" or "endogenous".

Exogenous activities are those whose operating levels are determined external to the region, e.g. steel mills operate at levels determined by national and international demands. Endogenous activities, on the other hand, are those whose operating levels are determined within the region, e.g. water treatment plants. This distinction is important, as the pollution generated is more a function of the operating level than the actual size of the activities.

The operating levels of endogenous activities are taken to be proportional to the demands placed on them by other activities in the region, both exogenous and endogenous. In SPACE these demands are measured in terms of the pollution transported to the endogenous activities. Not all endogenous activities can be characterized as receiving and processing pollution residuals, however. Thus, for electric power generating stations, and other such endogenous activities, dummy pollutants must be defined. These dummy pollutants are simply the demands, e.g. electric power demand. Like actual transported pollutants, these dummy pollutants are used primarily to determine the operating level of the receiving activities.

Through these various considerations, net pollution emitted in each grid square is determined. The final consideration in SPACE is the possible dispersion of the emitted residuals in air or water. This yields ambient levels of the residuals in each grid square.

As suggested by the foregoing discussion, SPACE, starting with an empty region grid for each analysis year, essentially creates a snapshot of the region for an average day during the year. This does not, however, mean that each year is analyzed independently. The carryover from one analysis year to the next is provided for in three ways. First, the data obtained from SEAS already reflects the impact of time on such items as economic productivity and growth, technological advances, population growth, changes in demand for industrial output, etc. Second, user designated policy changes remain in effect unless again changed. In particular, auto emission standards specified for one year, influence auto emissions for cars of that model year when analyzing subsequent years. Finally, land use patterns determined for one analysis year are a major consideration in specific activity location in subsequent analysis years. This approach in considering changes over time is most meaningful if the interval between analysis years is at least 3 years, and preferably 5 years or more.

SPACE System Structure

SPACE was originally conceived as a patchwork of existing models and data bases. It was not possible to strictly adhere to this concept, however, since existing elements were not always sufficiently compatible. As an alternative, the system was designed in modular form with usable existing elements adapted as modules and missing links developed specifically for the test version of SPACE. This design provides for relatively easy replacement of components as better models or data files become available.

The resulting modular system can be considered to consist of 13 components. Each of these will be discussed briefly.

SEAS Files

Reference has already been made to the use of SEAS data as the basis for SPACE analyses. Although much of the SEAS data is used in some form, two SEAS files are read directly by SPACE. These are the disaggregated economic projections and the pollution residual coefficients for the various economic sectors. The residual coefficients are estimates of pollution produced per unit of the activity, reflecting operating and/or production processes used, and, optionally, abatement processes used.

Modal City Files

The Modal City Files refer to the collection of data required as input to SPACE to describe the specific SMSA's being analyzed. Lest the idea of developing such files for each application scare off potential users, the original design of SPACE included the concept of Modal Cities (or Modal Regions). This concept envisions the development of a typology for the SMSA's, such that a small number of (actual or composite) SMSA's would be used to represent all SMSA's. These representative SMSA's would constitute the Modal Cities. A Modal City File would then be developed for each, and made part of the SPACE System. Efforts towards this end have been initiated recently, through an EPA contract with Urban Systems Research & Engineering, Inc. Currently SPACE contains only a single Modal City File, developed specifically for the test system.

Permanent Data Files

The major portion of the remaining inputs for SPACE will be referred to as the Permanent Data Files. These include data reflecting generalized behavior patterns, national averages, etc. Perhaps the most important items in these files are the descriptions of the economic sectors, including employment information, area requirements, etc. Other important data included in these files are pollution transformation factors and auto emissions standards.

MSPACE

The main program for the SPACE model is referred to as MSPACE. Its functions are to read the input data files, create a working data base, sequence the analysis through the designated analysis years, sequence the execution of assessment modules for each analysis year and create history files for possible future use. The design of this program is such as to permit relatively independent design and operation of the other component modules.

OVRIDE

A major design feature of SPACE is the means for introducing environment related policy. Subroutine OVRIDE serves this function. At the start of each analysis year, following the automatic updating of the working data base, SPACE allows the user to specify a broad spectrum of modifications reflecting new policies. These range from simple speed limit changes to more complex land use constraints.

Activity Allocation

The first of the major submodels executed each analysis year is the activity allocation module. This submodel distributes units of the various activities (population, specific industries, commercial activities, etc.) among the grid squares of the region. In dispersing a given activity an attractiveness index, relative to that type of activity, is calculated for each grid square. Within the constraints of minimum activity size, available land, and local policy, each activity is distributed in proportion to the size of the index. The total number of units distributed is essentially that implied by the SEAS projections. Where the minimum size is relatively small in comparison to total sector size, as in the case of housing, the resulting allocation will be highly dispersed. Where the minimum size is large, such as with heavy industry, the allocation will be more concentrated.

The attractiveness indices, which are the major bases for the allocation process, consider a wide range of grid square characteristics. These include accessibility, historical land use, distance from the central business district, the proximity of related activities and, if pertinent, the proximity of an employment base. The importance assigned each such attraction factor is varied with the type of activity being allocated.

Transportation

The transportation module operates directly on the results of the activity allocation module. Associated with each located activity are a number of trip ends, based on the activity type and size. These trip ends include those for work trips, business trips, shopping and recreation trips, freight pick-up and delivery, etc. The trips associated with each pair of trip ends are then categorized by type - auto, bus, rail transit, etc. through consideration of the local modal split. This modal split is determined from existing facilities, established patterns and local policies which encourage or discourage use of specific modes.

The trips themselves, specifically the vehicle miles traveled (VMT), are then distributed over the grid squares in a manner similar to the distribution of activities. Grid square attractiveness for trip miles is based on facilities available in the grid square (e.g. highway lane-miles, bus seat-miles, etc.), plus the number of trip ends located in or adjacent to the grid square. Finally the transportation module determines the average vehicle speeds in each grid square by considering legal speed limits and congestion implied by the ratio of the VMT distribution to highway capacity.

Pollution

The SPACE pollution module has been built around the Georgetown University IMMP Model.[2] Its main function is to convert data in the SPACE data base so as to be compatible with IMMP input requirements. This module controls the execution of IMMP, but the IMMP model, as modified, for SPACE, controls the execution of other submodels within the pollution module.

IMMP

The IMMP Model primarily takes care of the pollution analysis and accounting, including the considerations of pollution transformation, transportation and dispersion. In addition it determines the operating levels of the endogenous activities. Some modifications have been made to the IMMP program for its use in SPACE. These primarily involve the use of IMMP to control the execution of other components, specifically MOBILE, STORM and MAPS.

The only significant modification made to the analysis in IMMP relates to the determination of net pollution emissions by endogenous activities. The basic IMMP Model treats such emissions as being directly proportional to the operating level of the activity. As modified for SPACE, the net emissions from endogenous activities also reflect the mix of pollutant residuals received.

MOBILE

Subroutine MOBILE was developed to compliment IMMP, since the basic IMMP Model is limited in its ability to treat mobile pollution source emissions. This routine determines net emissions from motor vehicles in each grid square, and then passes the results to IMMP for inclusion in grid square totals. MOBILE considers both trip end and running emissions. It considers the mix of vehicle types, fuels used and average speeds. It further reflects emission standards and age distributions of the vehicles, which affect emission control quality.

STORM

One source of water pollution, not reflected in the other components discussed is the runoff from rain or melting snow. Since other analyses in SPACE reflect an average day during each analysis year, direct integration of this type pollution would not be meaningful. To handle this consideration, the Corps of Engineers' STORM Model[3] was adapted. This model analyzes the precipitation history in a region for a full year. It isolates precipitation/runoff events and determines the pollution content of the runoff for each event. It further considers treatment of the runoff (in a quantitative sense only) and possible storage and overflow of runoff awaiting treatment.

For purposes of SPACE analyses, STORM has been modified to isolate the results for an average rain day and a worst rain day. The levels of overflow and treatment thus determined are passed back to IMMP as amounts of pollution residuals dumped directly into streams and amounts transported to water treatment plants, respectively.

To accommodate this use of STORM, IMMP was further modified. IMMP now determines the remaining capacity of the water treatment plants, which it passes to STORM. Upon receiving the results of the STORM analysis, IMMP produces three sets of water pollution results - one for an average dry day, one for an average rain day and one for a worst rain day.

MAPS

The output formats incorporated in the basic IMMP and STORM models were not felt to adequately meet the needs of SPACE System users. As a result a general purpose routine was developed to produce rectangular grid displays, showing appropriate data for each grid square in the region. This routine, referred to as MAPS, is used to display a wide variety of SPACE output, including the net emissions and ambient levels of individual pollution residuals in each grid square.

History Files

The last of the major SPACE System components are the History Files. Following the analysis for each year, the working data base is copied to a semi-permanent History File. This feature allows the user to efficiently analyze variations of previous runs. Thus following a run involving 5 analysis years, the user may desire to rerun the situation with specific policy modifications introduced at the start of the third analysis year. This would be accomplished by using the History File created at the end of the second year to recreate the data base as it existed. The policy modifications would then be entered, and SPACE would be executed for only the last three analysis years.

SPACE Run Preparation

The mechanics of actually using the SPACE System can be very simple or relatively complex, depending on the degree of complexity associated with the policy options to be analyzed. Because of the variety of permanent files incorporated in the system, the use of SEAS Files and the anticipated existence of the Modal City Files, required user input, other than policy descriptions, is minimal. These include designation of analysis years, the Modal City File to be used and, if pertinent, the History File to be used for restart runs.

User specified policies are entered by modifying data in the working data base. The complexity involved in entering such policies is somewhat reduced by using a variable format approach for designating modifications. Thus, the user need only be concerned with the specific items to be changed. It is in the determination of items to be changed and, to a lesser degree, the new values to be introduced that the complexities arise. The test system has been designed to give the user maximum freedom in selecting policies to be analyzed. Thus there is no shopping list of options for the user to select from. Rather there is a list of factors that can be changed, e.g. speed limits, auto emission standards, abatement process effectiveness, etc. The user must translate his policy choice into value changes for one or more of the factors.

The various computer files that constitute the SPACE Test System all exist on a single EPA disk volume located at the Optimum Systems, Inc. (OSI) facility in Rockville, Maryland. To further aid users in run preparation, all pertinent files, including sample JCL instructions, have been stored so as to permit data input and job execution from remote terminals using the WYLBUR language. A draft users guide[4] for the test system is available for those desiring more details on this aspect of the system.

Summary

This, then, is the SPACE System - a collection of computer models and data bases capable of further disaggregating the determinations from SEAS, in such a way as to allow analysis of the impact on SMSA's of various local policies. It is a highly flexible system which, although intended primarily for the study of environmental pollution, can be used to study a variety of environment-related phenomena.

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RIBAM, A GENERALIZED MODEL FOR RIVER BASIN WATER QUALITY MANAGEMENT PLANNING

Richard N. Marshall, Stanley G. Chamberlain, Charles V. Beckers, Jr.
Environmental Systems Analysis
Oceanographic & Environmental Services
Raytheon Company
Portsmouth, Rhode Island

ABSTRACT

To meet water quality objectives in streams and rivers, a need arises for systematic analysis of alternative pollution abatement strategies. The computerized mathematical model, RIBAM (RIver BAsin Model), predicts water quality for 17 constituents, including DO, carbonaceous BOD, and parameters that represent nitrification and photosynthetic processes. Predicted water quality profiles throughout the basin for varying sets of waste loads and flow regimes can be compared with each other and with desired water quality goals. RIBAM is suited for determining the waste load allocations necessary for achieving water quality standards in rivers. A unique calibration method, based on open-channel hydraulic equations, for an exponential relationship between stream velocity and flow is presented.

The basic assumptions of RIBAM are that steady-state conditions exist and that the concentrations of water quality parameters are well mixed, varying only in the longitudinal direction of the stream. The application of RIBAM to the Beaver River Basin, including the Mahoning River, in Ohio and Pennsylvania is discussed.

BACKGROUND

RIBAM was developed by Raytheon Company under a project sponsored by the US Environmental Protection Agency to provide a verified, computerized mathematical model of the water quality in selected portions of the Beaver River Basin. RIBAM is a major modification of the DOSAG model.[1] In most cases, predicted values of water quality parameters at several Basin locations agreed with previously measured values during three simulated time periods.

RIBAM can be used by EPA, state and local agencies, and consulting firms for basin-wide water quality planning, in accordance with PL 92-500, the Federal Water Pollution Control Act Amendments of 1972. Raytheon held a model training seminar for the relevant agencies in Ohio. RIBAM is presently being used by the EPA Region V Michigan-Ohio District Field Office in Cleveland in an ongoing project to determine waste load conditions that most favorably meet water quality objectives in the Mahoning River, Ohio.

MODEL ASSUMPTIONS

In RIBAM, it is assumed that steady-state consitions exist in which the basin conditions are invariant with time. The basin conditions include the various effluent waste loads, stream flow, velocity, depth, and the model parameters, such as reaction rates and coefficients. Basin conditions can vary spatially, but only along the longitudinal direction of the stream. The water quality constituents modeled in RIBAM are assumed to have uniform values throughout any cross section of the stream at any given basin location.

BASIN NETWORK

RIBAM analyzes a river basin as a network consisting of the following four basic components:

Junction- confluence between two streams within the river basin.

Stretches - length of river between two junctions.

Headwater Stretches - length of river from a headwater to its first junction with another stretch (either headwater or normal).

Segments or Reaches - subunits of length that comprise a stretch (either headwater or normal).

In RIBAM, segments are defined such that the model parameters are assumed to be invariant throughout the length of the entire segment. At the head of each segment, new values of model parameters can be defined and additional flows and waste loads may enter the stream. Figure 1 demonstrates the modeling network for the RIBAM application to the Beaver River Basin.

SOLUTION TYPES IN RIBAM

The in-stream reactions that effect the concentrations of the 17 water quality parameters in RIBAM are represented by differential equations.

All of the differential equations have analytical solutions, which are computed in a piecewise continuous manner along the entire length of the river basin network. More specifically, a mass balance is computed as additional flows and waste loads enter the stream at the head of a segment. The solution for concentration of each water quality parameter is then computed for the length of the segment. The concentration at the downstream end of the segment is then an input to the mass balance at the head of the next down-stream segment.

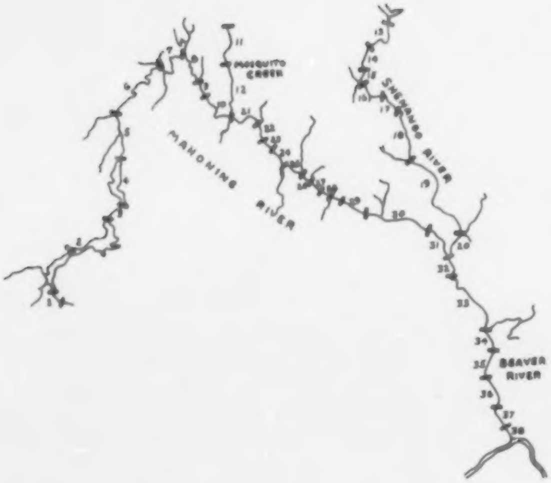

Figure 1. RIBAM Segmentation Network for Beaver River Basin

The differential equations and analytical solutions of the water quality parameters can be categorized into three types:

conservative

non-conservative, non-coupled

non-conservative, coupled

The conservative solution defines the concentration of the water quality parameter as being constant throughout the segment. The conservative equation is:

$$\frac{dC}{dt} = 0 \qquad (1)$$

where C = concentration of water quality parameter (usually mg/1)

t = time (days)

The conservative solution is:

$$C(t) = C_o \qquad (2)$$

where C_o is concentration at the head of the segment after the mass balance is computed (i.e., at time equal to zero) and t is time of travel through the segment.

The conservative parameters, or those parameters whose concentrations are defined by the conservative solution, are:

Sulfates
Manganese
Iron
Total Nitrogen
Dissolved Solids
Lead
Chlorides

In RIBAM, the mass exchange at the head of a segment is categorized according to three source types; 1) tributary sources, 2) municipal sources (discharge of treated municipal sewage), and 3) industrial sources. For each source type and each segment, the RIBAM user may select one flow value and one concentration value for each water quality parameter. If multiple sources of a single type are located at a segment head, flow and concentration must be combined externally for use in RIBAM. Tributary and municipal source types are similar because they represent flow and mass additions to the system. They are distinguished mainly to facilitate easier model use and interpretation of results. The tributary source type can be used to represent a withdrawal, by specifying a negative flow value. The industrial source type represents the mass added to water that is circulated through a facility for use in its industrial processing. The mass balance equation is:

$$C_o = \frac{C_sQ_s+C_1Q_1+C_2Q_2+C_3Q_3}{Q_s+Q_1+Q_2} \qquad (3)$$

where:

Q_s = stream flow entering from the upstream reach (cfs)

Q_1 = flow added by tributary sources (cfs)

Q_2 = flow added by municipal wastewater sources (cfs)

Q_3 = flow passing through industrial sources (cfs)

C_s = concentration of parameter at downstream end of the upstream segment (usually mg/l)

C_1 = concentration of parameter in tributary streams (usually mg/l)

C_2 = concentration of parameter in municipal wastewater sources (usually mg/l)

C_3 = net change in concentration between intake and discharge of industrial process water (usually mg/l)

The equation for the non-conservative, non-coupled solution is:

$$\frac{dC}{dt} = -KC \qquad (4)$$

where K is the reaction rate of the constituent.

The solution to equation (4) is:

$$C(t) = C_oe^{-Kt} \qquad (5)$$

In RIBAM, the following constituents are defined by the non-conservative, non-coupled solution:

Phosphorous
Ammonia Nitrogen
Cyanides
Phenols
Carbonaceous BOD
Coliforms

The non-conservative, coupled parameter equation links the constituent in concern with one or more other constituents. A unique equation and analytical solution exists for each of the following coupled parameters:

Nitrite Nitrogen
Nitrate Nitrogen
Chlorophyll a
Dissolved Oxygen (DO)

The relationships among constituents for the coupled parameters is shown in Table 1.

TABLE 1. RELATIONSHIPS AMONG COUPLED PARAMETERS

COUPLED PARAMETER	COUPLED TO
Nitrite Nitrogen	Ammonia Nitrogen
Nitrate Nitrogen	Nitrite Nitrogen Ammonia Nitrogen
Chlorophyll a	Phosphorous Nitrate Nitrogen Nitrite Nitrogen Ammonia Nitrogen
Dissolved Oxygen	Iron Nitrite Nitrogen Ammonia Nitrogen Carbonaceous BOD Chlorophyll a

The mathematical relationships among coupled parameters represent the natural processes of nitrification, bacterial oxidation of organic material, and photosynthesis. The equation for DO also includes terms for reaeration and benthic demand. Reference 2 presents the mathematical form for each coupled parameter.

The reaeration coefficient, K_{17}, may be specified for each reach, or it may be computed by:

$$K_{17} = \frac{A*V^B}{D^C} \qquad (6)$$

where V = stream velocity (fps)
D = stream depth (feet)

and A, B, and C are coefficient values, which have been determined for previous field studies[3]. RIBAM also predicts reaeration at dams[2].

CALIBRATION OF THE MODEL

In simulating water quality in a river basin for a previously observed time period, the predicted values of the model are compared with measured values. The model is calibrated to the river basin when agreement is attained between predicted and measured values.

Each reach of the stream has a unique set of model parameters, reaction rates and coefficient values, that affect the predicted values. The model is calibrated by adjusting the model parameter values. The sensitivity of model predictions to the model parameters describes the relative change in predicted values due to variations in the model parameter values. Figure 2 demonstrates the comparison between predicted and measured values for the calibration of dissolved oxygen in the Mahoning River, Ohio for a time period in July-August 1971. The calibrated model is usually verified with a favorable comparison of predicted and measured values for simulations using the calibrated model parameter values for one or more previously observed time periods.

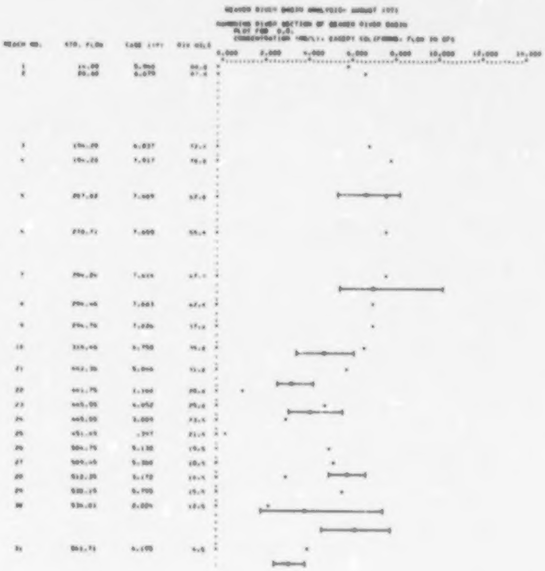

Figure 2. Comparison of Predicted and Measured Values of Dissolved Oxygen, Mahoning River

The stream velocity is an important term in RIBAM, because it is inversely related to t, the time of travel through a reach. For non-conservative, non-coupled parameters, the amount of reactant removed by natural processes is exponentially related to t (see equation (5)). Similarly, the mass lost or gained by coupled parameters is sensitive to the value to t.

The velocity of a reach is estimated by:

$$V = aQ^b \qquad (7)$$

where Q = stream flow (cfs)
and a, b are coefficient values. The values may be determined from a statistical analysis of several flow-velocity observations within the reach. Frequently, observations are limited to a time of travel measurement over a length of stream for one flow condition.

Consequently, a method is developed to determine the coefficients from limited data. This method applies the basic hydraulic equations for open channel flow to obtain several pairs of velocity and flow values for each reach. A statistical regression is then applied to these values to determine the coefficients of equation (7). The first hydraulic equation[4] is:

$$Q = \frac{1.49}{n} AR^{2/3} S^{1/2} \qquad (8)$$

where:

A = cross sectional area (ft^2)

R = cross sectional area divided by wetted perimeter (hydraulic radius, ft)

S = slope or energy gradient

n = Manning coefficient

In this method, rectangular stream cross-sections are assumed, yielding the following definitions:

$$R = \frac{DW}{W+2D} \qquad (9)$$

where W = stream width (ft)

$$\text{and} \quad A = DW \qquad (10)$$

Upon substitution, equation (8) becomes

$$-K^3W^5D^5+4Q^3D^2+4WQ^3D+Q^3W^2 = 0 \qquad (11)$$

$$\text{where } K = \frac{1.49}{n} S^{1/2}$$

Depth is the only unknown quantity in equation (11) if Q is defined as a measured flow value or treated as an independent variable. Equation (11) is a polynomial in D, which can be solved numerically using Newton's method.

When depths have been determined by solving equation (11), the velocities are computed using the hydraulic equation[4].

$$V = \frac{1.49}{n} R^{2/3} S^{1/2} \qquad (12)$$

To determine flow-velocity pairs, equation (11) and (12) must be solved a sufficient number of times for accuracy in the statistical regression. The independent variable, flow, should be varied over the expected range of values. Widths, which are assumed to be invariant over the range of flows, and the slopes must be estimated from detailed maps or other sources. If a measurement of average velocity (or time of travel) has been made for the reach, the value of n can be found by iteratively computing equations (11) and (12) and determining which value is in the best agreement with the measured velocity. In the absence of velocity measurements, an engineering estimate of n must be made.

The flow-velocity pairs generated from equations (11) and (12) are fitted to the curve defined by equation (7) by statistical regression techniques. The resulting coefficients can be used for velocity predictions in RIBAM simulations. The method offers the advantage of a simple velocity prediction equation that is based on the physical characteristics of the reach and that requires limited or no observational data on velocity.

SENSITIVITY ANALYSIS

Results of a sensitivity analysis demonstrate the numerical significance of model parameters to the RIBAM predictions. For example, the percent change of a predicted value may be compared with similar percent changes in model parameter values that affect the prediction. RIBAM sensitivity analysis results for the Beaver River Basin are reported in reference 2.

MODEL APPLICATIONS

Upon calibration of RIBAM to a particular basin, the model can be used to predict water quality for projected conditions. RIBAM is a simple, effective tool for determining waste load allocations for point sources in a river basin. The model can estimate water quality profiles for varying effluent loadings, which may be due to changing sewered population, increased treatment, or addition of a new discharge facility. The water quality can be simulated for different environmental conditions, such as stream flow and water temperature. RIBAM has been used by USEPA personnel to predict water quality for projected conditions in the Mahoning River.

USER-COMPUTER INTERFACE

RIBAM, like other computer models, requires the user to learn data deck input formats and model outputs. The RIBAM input/output is straightforward, and fully documented[2]. Figure 3 presents a typical printout for RIBAM water quality predictions. The computation time and costs for RIBAM are relatively low compared to water quality models that require numerical solutions, such as finite difference techniques.

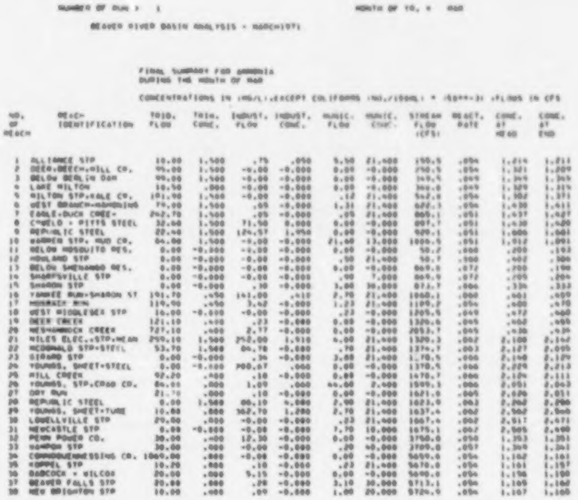

Figure 3. Typical RIBAM Final Summary Table for a Non-Conservative, Non-Coupled Parameter.

CONCLUSIONS

RIBAM is useful for the basin-wide water quality planning function. Predicted water quality profiles for different basin conditions can be analyzed to aid in determining the waste load conditions that are most suitable to the water quality objectives of the basin. Coefficients for the velocity prediction equation can be determined by a method that considers the physical characteristics of the stream and requires minimal observational data.

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COMPARISON OF EUTROPHICATION MODELS

By: John S. Tapp
Environmental Protection Agency
Technical Support Branch
Water Division
Region IV
Atlanta, Georgia

Summary

A complex mathematical model for simulating an aquatic ecosystem was compared with less complex models of the type developed by Vollenweider to see if utilizing the sophisticated mathematical approach adds to the decision making ability in comparison to the less complex models. The reservoir used for comparison was Lake Harding on the Chattahoochee River in Georgia and Alabama. Data collected by the EPA National Eutrophication Survey on 66 Southeastern water bodies were used to test the Vollenweider type models. Results indicate that for Lake Harding either approach would give comparable results in terms of the decision to limit point source phosphorus to the reservoir.

Introduction

The problem of eutrophication has traditionally been a difficult one for regulatory agencies. The complex interactions that occur in a reservoir or lake generally cannot be easily defined to the point where assessing the impact of a point or nonpoint wastewater source discharge on a lake can be made with detailed accuracy. Over the years, three basic approaches have evolved for use by agencies in order to make decisions concerning limitations of nutrients, namely nitrogen and phosphorus, into aquatic systems. The three approaches are (1) complex reservoir models which try to simulate the complex interactions that occur within a water body; (2) a more simplistic approach which relates the input of phosphorus to a water body or the concentration of phosphorus in a water body with its physical properties; and (3) a very simplistic mass balance approach. Realizing the limitations of the very simplistic mass balance, the two approaches in general use today are the complex reservoir model and the approach relating an input or in-lake concentration of phosphorus to some physical characteristics of the water body (commonly called the Vollenweider approach).

From a scientific standpoint, the best approach would be the complex modeling approach which, if carried to an extreme, would attempt to represent accurately the complex interactions that occur within a lake or reservoir. However, in practical terms, the ability to represent these complex interactions is limited because some interactions have not yet been identified and some that are known cannot readily be measured. Very extensive and expensive research and data collection programs could attempt to accurately represent all identified and measurable constituents and interactions occurring in the complex ecologic system. However, the collection of this massive amount of data is usually infeasible within budgetary restrictions; therefore, a common approach used is to define the major interactions and base the model upon these interactions. A minimum data collection program to calibrate one of these complex models representing only the major interactions is still very expensive. The question is whether going to a relatively sophisticated mathematical approach really adds to the decision making ability as compared with the less complex Vollenweider approach. This paper attempts to address this question in relation to one reservoir in a Southeastern United States setting.

Complex Reservoir Model-EPAECO

An example of a reservoir model currently in use today is one developed for EPA by Water Resources Engineers[1] and is known by the acronym EPAECO. The model was originally developed for the Office of Water Resources Research (USDI) and simulates the temporal variation of vertical water quality and biologic profiles over an annual cycle in response to meterologic conditions, tributary conditions, and reservoir releases. In reality, an aquatic ecosystem has a delicate and stable balance of many different aquatic organisms and water quality constituents. The reservoir ecologic model solves a set of equations which represent only the more significant interactions of the reservoir biota with water quality. The reservoir ecologic model EPAECO simulates the hydrodynamic water quality and biological responses of reservoirs to tributary inputs and environmental energy exchanges in reservoir releases.

Vollenweider Approach

The other basic type of model in use today is a nutrient budget model for phosphorus derived by Vollenweider[2]. As indicated in Figure 1, Vollenweider plotted phosphorus loading in grams per square meter per year versus the mean depth divided by the retention time of a lake. Vollenweider then empirically defined a basic loading tolerance for the case where the mean depth divided by the retention time was much less than one. Using the solution to the equation, the loading tolerance lines were projected throughout the commonly encountered ranges of mean depth divided by retention time. The lower line was called the permissible limit and the upper line was called the dangerous limit and was defined as twice the permissible limit. The permissible limit was said to separate oligotrophic and mesotrophic lakes and the dangerous limit was to separate mesotrophic and eutrophic lakes. Vollenweider and Dillon[3] furthered the Vollenweider approach using the steady state solution to the model. If dangerous and permissible lines are drawn as shown in Figure 2, the trends represent equal predictive phosphorus concentrations. This model indicates that the prediction of the trophic state of the lake is based on a measure of the predictive phosphorus concentration in the lake rather than on the phosphorus loading and is called the Dillon model.

Larsen and Mercier[4] expressed Vollenweider's mass balance model in terms of concentration. The Larsen-Mercier curves relate the steady state lake and mean input phosphorus concentrations. Larsen and Mercier selected values of 10 and 20 micrograms

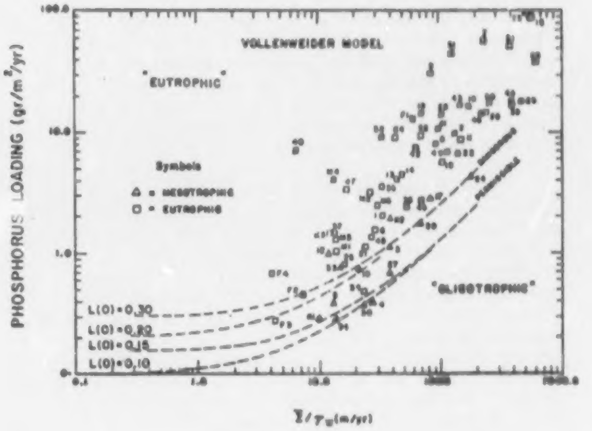

FIGURE 1. The Vollenweider Model and Data from Southeastern Lakes and Reservoirs

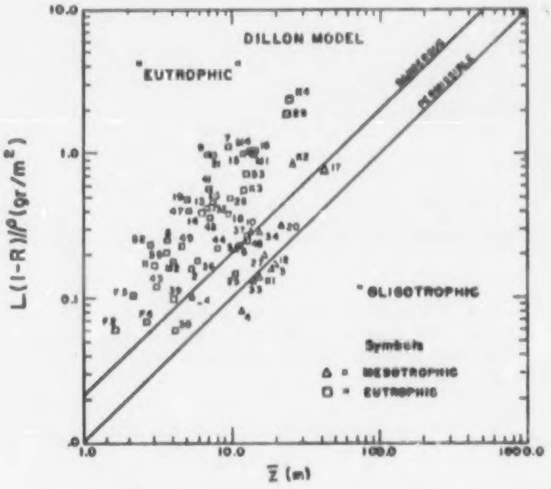

FIGURE 2. The Dillon Model and Data from Southeastern Lakes and Reservoirs

of phosphorus per liter to delineate the oligothopic, mesotrophic and eutrophic states. These values were selected based on studies in the literature suggesting that springtime concentrations of total phosphorus in excess of 20 μg/l were likely to produce average summer chlorophyll concentrations of 10 μg/l or greater. Larsen and Mercier's curves are shown in Figure 3.

Physical Setting-Lake Harding

The reservoir used to compare the models described above was Lake Harding, also known as Bartlett's Ferry Reservoir, and is located on the Chattahoochee River about 120 river miles downstream from Atlanta, Georgia and approximately 286 river miles upstream from the confluence of the Chattahoochee and Flint Rivers. The general location is

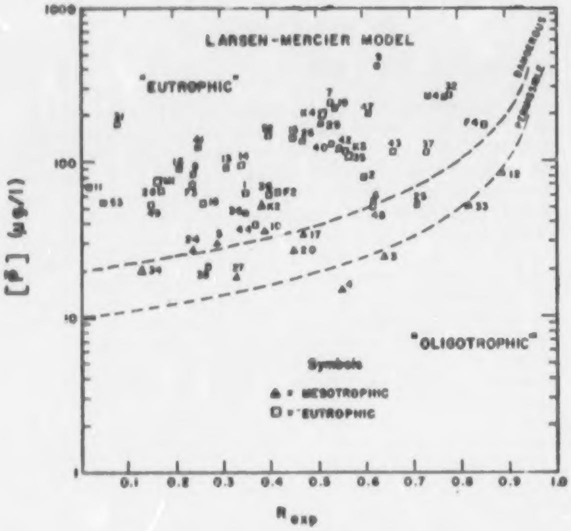

FIGURE 3. The Larsen-Mercier Model and Data from Southeastern Lakes and Reservoirs

shown in Figure 4. This reservoir was chosen because Water Resources Engineers[5] under contract to EPA had calibrated the reservoir ecologic model EPAECO on the reservoir.

From a eutrophication standpoint, Lake Harding is very advanced, i.e., anaerobic conditions prevail in the lower depths of the reservoir during the summer months, productivity is high, and the water is turbid. Since the time EPAECO was calibrated on Lake Harding, a new reservoir immediately upstream has been impounded. Therefore, the projections utilized in this paper are merely to compare the results from the various models and essentially have no application in terms of real effluent limitations to be established, except where parallels can be drawn between Lake Harding and the new upstream reservoir.

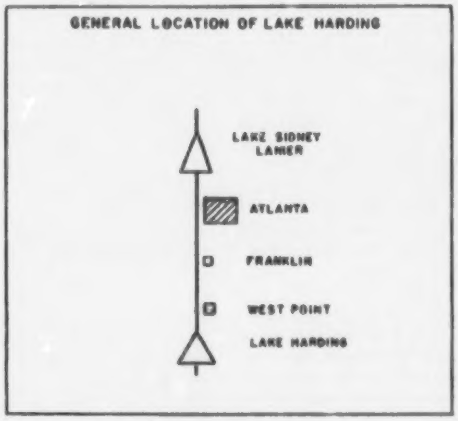

FIGURE 4. The Location of Lake Harding

Results and Discussion

Vollenweider Type Models

Gakstatter et al.^{6} summarized the results of the 3 Vollenweider type models in relation to data collected by the National Eutrophication Survey on 23 water bodies most of which were located in the Northeastern and North Central United States. The study concluded that based on the trophic state classification developed by the National Eutrophication Survey, the models developed by Dillon and Larsen-Mercier fit the data much better than Vollenweider's model. The Vollenweider model was probably less precise because unlike the Dillon and Larsen-Mercier models it only considers total phosphorus loading without regard to in-lake processes which reduce the effective phosphorus concentration.

Gakstatter and Allum^7 also compared the Vollenweider, Dillon and Larsen-Mercier models with data collected by the National Eutrophication Survey from 53 water bodies in the states of Georgia, North Carolina, South Carolina and Alabama. The data of Gakstatter and Allum for the 53 water bodies and additional data from 13 other Southeastern water bodies also collected by the National Eutrophication Survey in the states of Kentucky, Florida and Mississippi are shown in Figures 1, 2 and 3. The trophic state index used for these data was that developed by the National Eutrophication Survey. Figures 1, 2 and 3 indicate that for the 66 water bodies all three of the Vollenweider type models generally fit the data. The names of the water bodies and the hydraulic retention time of each are shown in Table 1.

TABLE 1. KEY TO LAKES SHOWN IN FIGURES 3, 4 AND 5.
HRT = hydraulic retention time in years

Lake	No.	HRT	Lake	No.	HRT	Lake	No.	HRT
Allatoona	1	0.23	Lookout Shoals	23	0.02	Gantt	45	0.02
Blackshear	2	0.04	Mt. Island	24	0.03	Pickwick	46	0.02
Blue Ridge	3	0.08	Norman	25	0.65	Purdy	47	0.30
Burton	4	0.08	Rhodhiss	26	0.06	Martin	48	0.08
Chatuge	5	0.91	Santeetlah	27	0.08	Guntersville	49	0.08
Clark Hill	6	0.37	Tillery	28	0.08	Lay	50	0.04
Harding	7	0.04	Waterville	29	0.08	Mitchell	51	0.01
High Falls	8	0.04	W. C. Bowen	30	–	Weiss	52	0.04
Jackson	9	0.08	Fishing Creek	31	0.02	Wilson	53	0.02
Nottley	10	0.63	Greenwood	32	0.22	Monroe	F1	0.03
Seminole	11	0.02	Hartwell	33	0.92	Kissimmee	F2	0.24
Sidney Lanier	12	1.49	Keowee	34	1.10	Istokpoga	F3	0.08
Sinclair	13	0.15	Marion	35	0.12	Tohopekaliga	F4	0.69
Walter F. George	14	0.13	Moultrie	36	0.11	Dale Hollow	K1	1.49
Blewett Falls	15	0.02	Murray	37	0.95	Cumberland	K2	0.70
Badin	16	0.04	Robinson	38	0.10	Barren River	K3	0.94
Fontana	17	0.49	Saluda	39	0.41	Herrington	K4	0.50
Hickory	18	0.09	Secession	40	–	Sardis	M1	1.10
High Rock	19	0.07	Wateree	41	0.07	Ross Barnett	M2	0.13
Hiwassee	20	0.32	Wylie	42	0.11	Grenada	M3	1.10
James	21	0.57	Bankhead	43	0.03	Enid	M4	1.12
Junaluska	22	0.04	Holt	44	0.02	Arkabutla	M5	0.29

To investigate the effect of hydraulic retention time on the fit of the data for the 66 Southeastern water bodies, those with hydraulic retention times of less than or equal to 0.08 years (30 days) were compared with the Vollenweider, Dillon, and Larsen-Mercier models as shown in Figures 5, 6 and 7. Those with hydraulic retention times of greater than 0.08 years were compared with the 3 models as shown in Figure 8, 9 and 10. The results indicate that the three models are generally applicable for water bodies with both long and short mean hydraulic retention times.

Lake Harding was one of the water bodies sampled by the EPA National Eutrophication Survey^8. Characteristics of the reservoir determined by the National Eutrophication Survey are shown in Table 2. Annual phosphorus loads are shown in Table 3. The survey found that for the most part Lake Harding was phosphorus limited, although the most upstream station in the lake which was nearer the relatively small point source wastewater discharges tended to be nitrogen limited. Because the National Eutrophication Survey considered only point sources within a 25-mile radius, a majority of the nonpoint phosphorus load in the Chattahoochee River as shown in Table 3 is from wastewater treatment plants in the Atlanta metropolitan area.

Marlar and Herndon^9 have estimated the Atlanta area point source input of phosphorus to the Chattahoochee River as 1,006,992 kilograms per year, which indicates that Atlanta point sources account for approximately 76 percent of the total phosphorus load in the Chattahoochee River tributary and 72 percent of the total phosphorus input to Lake Harding. Nonpoint source inputs to the Chattahoochee River tributary represent 22 percent of the total phosphorus in the river. The yearly average phosphorus loading to Lake Harding from the National

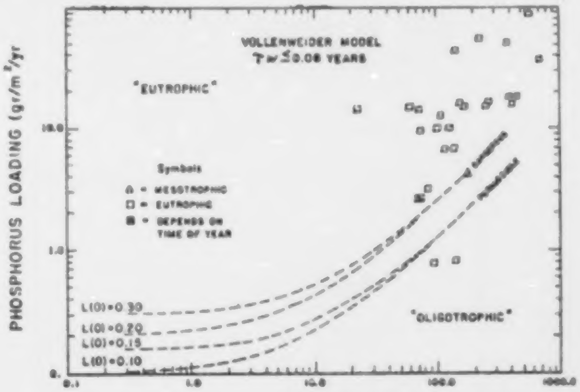

FIGURE 5. The Vollenweider Model and Data from Southeastern Lakes and Reservoirs with Hydraulic Retention Times Less than or Equal to 0.08 Years

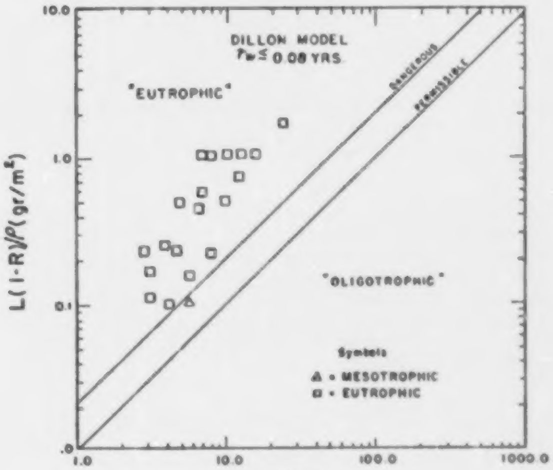

FIGURE 6. The Dillon Model and Data from Southeastern Lakes and Reservoirs with Hydraulic Retention Times Less than or Equal to 0.08 Years

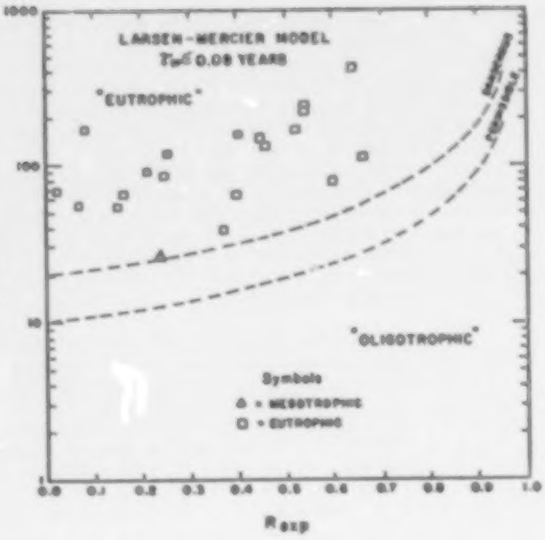

FIGURE 7. The Larsen-Mercier Model and Data from Southeastern Lakes and Reservoirs with Hydraulic Retention Times Less than or Equal to 0.08 Years

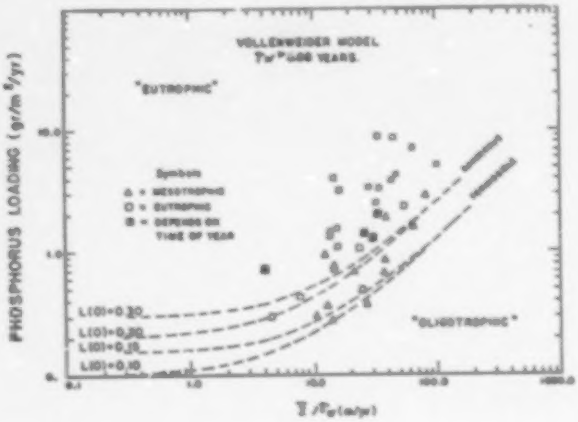

FIGURE 8. The Vollenweider Model and Data from Southeastern Lakes and Reservoirs with Hydraulic Retention Times Greater than 0.08 Years

TABLE 3. CHARACTERISTICS OF LAKE HARDING		
MORPHOMETRY		
Surface Area: 23.67 square kilometers		
Mean Depth: 9.4 meters		
Maximum Depth: 33.9 meters		
Volume: 222.098x10^6 cubic meters		
Mean Hydraulic Retention Time: 14 days		
TRIBUTARY	DRAINAGE AREA (Km^2)	MEAN FLOW (m^3/sec)
Chattahoochee River	9,479.4	165.3
All Others	1,478.9	20.6
TOTAL:	10,958.3	185.9
MEAN OUTLET FLOW		185.9

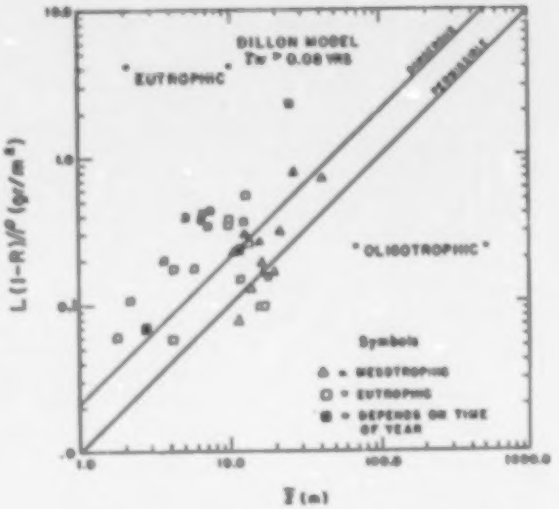

FIGURE 9. The Dillon Model and Data from Southeastern Lakes and Reservoirs with Hydraulic Retention Times Greater than 0.08 Years

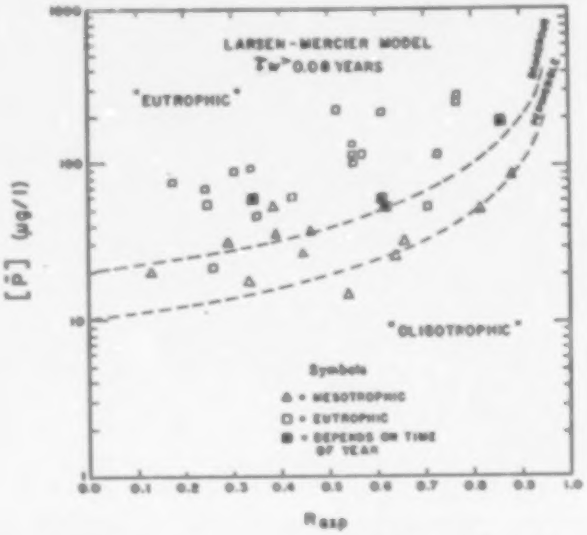

FIGURE 10. The Larsen-Mercier Model and Data from Southeastern Lakes and Reservoirs with Hydraulic Retention Times Greater than 0.08 Years

Eutrophication survey data was 58.74 grams/m^2/year based on total input. The calculated allowable loadings in grams/m^2/year to maintain dangerous and permissible in-lake concentrations based on the models of Vollenweider, Dillon, and Larsen-Mercier are shown in Table 4.

If 90 percent of the Atlanta point source contribution of phosphorus to Lake Harding were removed, the loading rate would be reduced to 20.45 grams/m^2/year, which is about twice the dangerous loading indicated by the Larsen-Mercier and Dillon models and about 3 times that indicated by the Vollenweider model. If 99 percent of all of the Atlanta point source phosphorus to Lake Harding were removed, the loading rate would be 15.36 grams/m^2/year which is beginning to approach the dangerous level of the Dillon and Larsen-Mercier models, but is still about 2.5 times that of the Vollenweider model. A cursory attempt was made to analyze other Southeastern water bodies sampled by the National Eutrophication Survey with phosphorus loadings in the 15 grams/m^2/year range and with physical characteristics similar to Lake Harding to see if this loading indicated an impairment of use of the water body. However, the analysis failed to reveal sufficient data upon which to base a conclusion.

TABLE 3. AVERAGE ANNUAL TOTAL PHOSPHORUS LOADING TO LAKE HARDING

INPUTS	Lb P/yr	% of Total
Chattahoochee River (nonpoint)	1,318,550	94.9
Other major tributaries (nonpoint)	36,430	2.6
Minor tributaries and immediate drainage (nonpoint)	3,000	0.3
Municipal STP's (point)	31,190	2.3
Industrial	Unknown	
Septic tanks	325	0.1
Direct precipitation	815	0.1
TOTAL	1,390,390	
OUTPUTS		
Lake Outlet	688,575	
NET ACCUMULATION	701,815	

TABLE 4. CALCULATED LAKE HARDING PHOSPHORUS LOADINGS (gr/m^2/year)
Present Loadings=58.74 gr/m^2/year

	VOLLENWEIDER	DILLON	LARSEN-MERCIER
Permissible	3.1	5.5	5.2
Dangerous	6.2	11.0	10.4

EPAECO

The reservoir model EPAECO utilizes concentrations of water quality constituents in the tributaries as input to the model. For the Lake Harding calibration, the only tributary considered was the Chattahoochee River because this was the only tributary on which any water quality data were available during the simulation period (July through December, 1973). Also, as shown in Table 3, the Chattahoochee River provides the majority of the phosphorus input to Lake Harding. The tributary water quality data available on the Chattahoochee River consisted of one sample per month for the six month study period. Daily tributary input concentrations to EPAECO were obtained by linear interpolation of the monthly data. Tributary concentrations of water quality constituents that were not measured during the monthly sampling were estimated based on the past experience of Water Resources Engineers.

In order that EPAECO simulate conditions with various phosphorus removal rates from point sources in Atlanta, a routine was written into the model to reduce the daily tributary concentrations to reflect point source removals. This was accomplished by taking the daily tributary concentration of phosphorus and daily flow and converting to pounds of phosphorus. The pounds of phosphorus assumed to be removed by 90% removal from the Atlanta point sources (based on yearly average loadings converted to daily average loadings) were subtracted from the instream pounds and the resulting number was converted back to concentration for input to the reservoir. On several days this calculation left no phosphorus for input to the reservoir. However, this was not believed significant due to the nature of the various estimates such as estimated yearly average point source loadings and interpolated daily instream concentrations.

The model is designed to simulate the reservoir for a one year period. The Lake Harding simulation included only day 202 (July 21) through day 365 (December 31). Accordingly, the same period was used in this study. As noted earlier, the average hydraulic retention time was approximately 20 days during the simulation period. Therefore, for the period of study the lake water theoretically exchanged about eight times, which should be enough to wash out initial conditions and allow the impact of the 90 percent point source phosphorus removal to be assessed.

The temperature stratification in the reservoir as calculated by EPAECO is shown in Figure 11 and the corresponding dissolved oxygen stratification is shown in Figure 12. Rather pronounced temperature stratification existed throughout much of the simulation period. Supersaturated surface dissolved oxygen concentrations and very low bottom dissolved oxygen concentrations were also exhibited throughout the majority of the simulation period. The simulation denoted by "1973 conditions" represents the best calibration of the model for the study period and is used as the base for evaluating conditions with phosphorus removal.

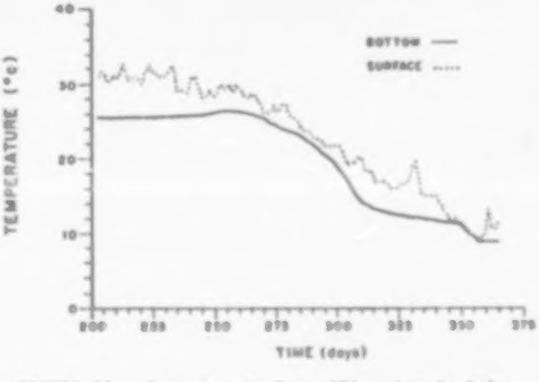

FIGURE 11. Temperature Stratification in Lake Harding as Calculated by the Reservoir Ecologic Model EPAECO

The changes in surface dissolved oxygen concentrations between 1973 conditions and the same conditions with 90 percent point source phosphorus removal are shown in Figure 13. Throughout the simulation period the dissolved oxygen concentration at the surface remained essentially the same after removal of point source phosphorus. The same was true for dissolved oxygen concentrations at the bottom of the reservoir. The orthophosphorus (as P)

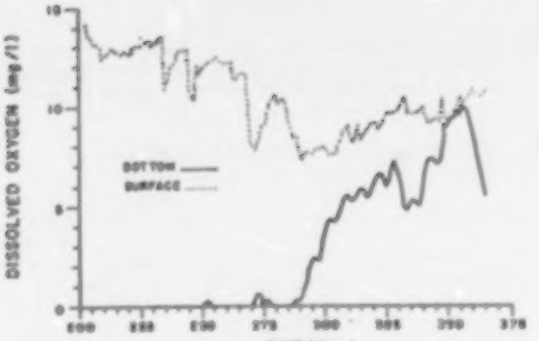

FIGURE 12. Dissolved Oxygen Stratification in Lake Harding as Calculated by the Reservoir Ecologic Model EPAECO

concentrations at the surface are shown in Figure 14 and the corresponding concentrations of green and blue-green algae at the surface are shown in Figures 15 and 16, respectively. As would be expected, lowering the orthophosphorus concentration to the reservoir resulted in an eventual lowering of surface orthophosphorus concentrations. The same trend was noted for orthophosphorus concentrations at the reservoir bottom. Phosphorus removal reduced the peaks in surface green algae concentration which would indicate lowering of concentrations during periods of algal blooms. The area differential under the two curves in Figure 15 indicates a 20 percent reduction in green algal biomass after point source phosphorus removal. Peaks in surface blue-green algae concentrations are also reduced indicating lower bloom concentrations and indicating a 35% reduction in biomass after point source phosphorus removal. The zooplankton concentrations at the surface were the same before and after point source phosphorus removal.

Figure 17 displays the total weight of the 3 types of fish on an areal basis throughout the simulation period and indicates that phosphorus removal would reduce the total weight of fish in the reservoir. The decline in total fish was due to a decline in the warmwater fish which cannot be readily explained based on model output. Also shown is a large growth of fish from day 250 to day 310 which is probably of the correct magnitude but not at the proper time.

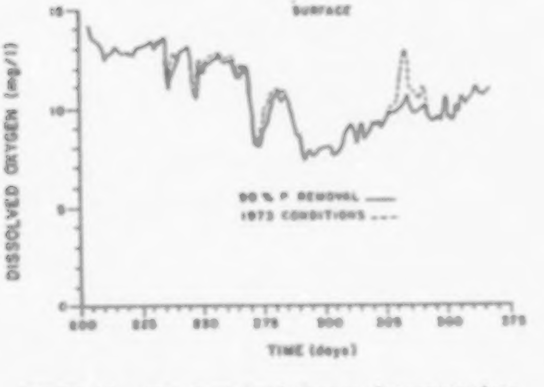

FIGURE 13. The Dissolved Oxygen Concentrations Before and After Point Source Phosphorus Removal as Calculated by EPAECO for Lake Harding

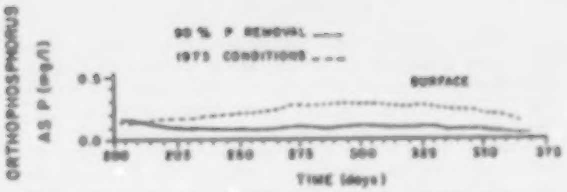

FIGURE 14. The Orthophosphorus Concentrations Before and After Point Source Phosphorus Removal as Calculated by EPAECO for Lake Harding

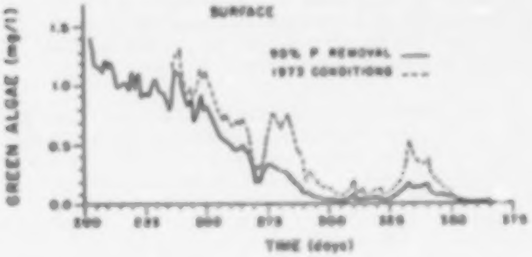

FIGURE 15. The Green-Algae Concentrations Before and After Point Source Phosphorus Removal as Calculated by EPAECO for Lake Harding

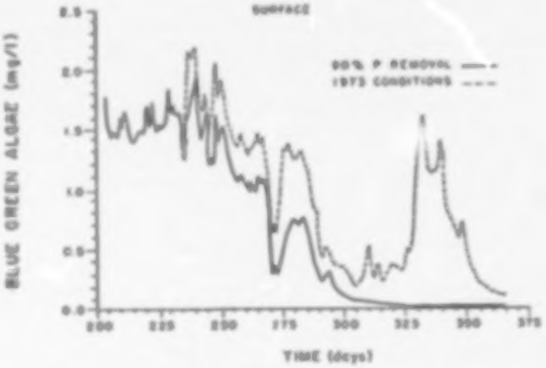

FIGURE 16. The Blue-Green Algae Concentrations Before and After Point Source Phosphorus Removal as Calculated by EPAECO for Lake Harding

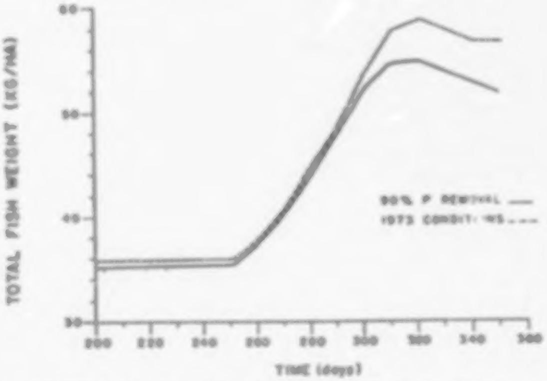

FIGURE 17. The Combined Weight of the Three Classes of Fish Before and After Point Source Phosphorus Removal as Calculated by EPAECO for Lake Harding

Conclusions

Based on the data collected by the EPA National Eutrophication Survey on 66 water bodies in the Southeastern United States, the Vollenweider model, the Dillon model, and the Larsen-Mercier model all have some merit when examining eutrophication problems. Since the Vollenweider model considers total phosphorus input to a water body and does not account for phosphorus in the outflow from the water body, it is the most conservative of the three for establishing load restrictions to a water body. The Vollenweider model should therefore be used as a first cut analysis in the absence of data. Where data exist to establish a phosphorus retention coefficient, the Larsen-Mercier and Dillon models should be used as a first cut to establish load restrictions to a water body.

The EPAECO model simulations indicate that with 90 percent point source phosphorus removal, yearly green and blue-green algal biomass would decrease by 20 percent and 35 percent, respectively. This should result in some improvement in the water quality in the reservoir even though the simulations showed no differences in dissolved oxygen before and after phosphorus removal. The results from using the Vollenweider, Dillon, and Larsen-Mercier models indicate that even with point source phosphorus removal the reservoir would still remain eutrophic. However, a closer examination indicates that 99 percent point source removal would reduce the loading rate to the same range as the dangerous rate calculated by the Dillon and Larsen-Mercier models. Therefore, intuitively, some improvement should result over a long term.

To make the Vollenweider type approach truly applicable to Southeastern water bodies, further work needs to be done to relate the trophic state of a given water body to an actual present or future impairment of water use in the water body. The trophic state classification presently used by the National Eutrophication Survey weighs heavily chemical parameters and turbidity. In Southeastern water bodies, these parameters are greatly influenced by the interactions with the clay based soils typical in the Southeast and may not give a true indication of the actual trophic state.

In terms of Lake Harding, either approach, EPAECO or the Dillon and Larsen-Mercier models, supports the conclusion that control of upstream point sources of phosphorus would be of benefit to the overall water quality in the lake. The conclusion is valid for the specific case examined, i.e., a relatively small lake with an extremely high phosphorus loading and a relatively small hydraulic retention time. Other lakes where sophisticated lake models have been constructed should be similarly tested to see if this conclusion is valid for the majority of impounded reservoir situations encountered in the United States.

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List of Symbols

$\bar{z}$ = mean depth (meters)

τ_w = hydraulic retention time (years)

L = phosphorus loading (grams per square meter per year)

R or R_{exp} = phosphorus retention coefficient (fraction retained)

ρ = hydraulic washout coefficient ($1/\tau_w$, years^{-1})

$[\bar{P}]$ = mean influent phosphorus concentration (micro grams per liter)

MANAGEMENT IN COMPETITIVE ECOLOGICAL SYSTEMS

Donald R. Falkenburg
School of Engineering
Oakland University
Rochester, Michigan 48063

1. Abstract

A competitive ecology is an essentially unbalanced system in which a weaker species is driven out of existence by a stronger competitor. Management policies which include selective harvest and replenishment alter the equilibrium states of such a system so that both the stronger and weaker members of the competitive system can coexist.

2. The Competition Equation

The Volterra competition model describes the growth dynamics of several species competing for the same environmental resource. Volterra[1] reasoned that if the depletion of the resource increases linearly with population size which in turn reduces the growth rate, and if each species has a different efficiency for utilizing the resource, then the growth equations have the following form:

$$\frac{dX_i}{dt} = X_i \left[\epsilon_i - \gamma_i \sum_{j=1}^{N} \alpha_j X_j \right] \quad i = 1,2....N \quad (1)$$

Although this quadratic interaction model may be simplistic, it does possess sufficient "richness" to predict the replacement of a "weaker" species by a "stronger" competitor - the so called competitive exclusion principle of Gause.[2] Volterra's competition model is one of a class of eco-system models which describe the interaction among several species. Scudo[3] presents an excellent summary of these models along with a well selected list of references to Volterra's work.

In order to understand the assumptions which underlie the Volterra and related competition models let us examine a situation in which two species are in a competitive environment. Let N_1 and N_2 be the size of the two populations which compete for a food supply F. The assumption that the growth of N_1 and N_2 are independent of the age structure of those populations renders to the model a significant simplification. It is important to realize that the preceeding statement does not imply age structure is absent from the population, but rather the population has attained a stable age configuration[4]; under such conditions the population can be modeled by an ordinary differential equation. The second important assumption is that the model is fundamentally deterministic. We know that the dynamic model of a population system reflects an aggregate interaction among individual members of the population - an interaction which arises from random encounters. If there are very few individuals then we must model such a system from a probabilistic perspective. If, on the other hand, there are many individuals within the population, it is often reasonable to construct a macroscopic model - a model which we use to project the size of a population and not the probability density function for the population size. The assumption that the model is macroscopic does not preclude that such a model may itself be subject to random disturbances.

The third and perhaps the most restrictive assumption is that the competing species which are being modeled are isolated. Simply stated it is not likely that one can ever observe a pure two-species interaction in nature; the complex ecological webs which exist attest to this. In fact, the growth of a single species may be affected by hundreds of other species. One way of dealing with this situation is to add disturbance inputs to the describing equations in an attempt to include the influence of species which are not explicitly represented in the model.

The competition model involves these three species - the two competitors and the resource (in this case, a food base) for which they compete. A dynamic model for such a three-species system is given in equation (2).

$$\begin{aligned} \frac{dN_1}{dt} &= -k_1 N_1 + q_1 F N_1 \\ \frac{dN_2}{dt} &= -k_2 N_2 + q_2 F N_2 \\ \frac{dF}{dt} &= k_f F - pF^2 - \alpha_1 F N_1 - \alpha_2 F N_2 \end{aligned} \quad (2)$$

The last of these equations describes the dynamics of the food base. The coefficient of growth k_f for the food base is assumed to be positive. The second term on the right hand side of this equation accounts for the reduction in the population growth due to the pressure of increasing population size. The remaining two terms account for the consumption of the resource by the two species. Here it is assumed that the per capita consumption increases linearly with the available food. In the first two equations, consumption of the food base leads to a linear increase in the per capita growth rate (this may occur through the reduction of the mortality rate, an elevation in the reproductive capacity or through a combination of both). Now, it is not necessary to assume that the relationships described above are linear; in fact within the last section of this paper an analysis is presented which is applicable to a generalized population interaction model. Finally, if one assumes that the characteristic response time of the food base is much smaller than the response times for the competing species, i.e., $k_f >> k_1$, k_2, then the dynamic equation representing the growth of the food base can be replaced by the quasi-static equation

$$F(k_f - pF - \alpha_1 N_1 - \alpha_2 N_2) = 0. \quad (3)$$

Using equation (3) to eliminate F from the first two equations in (2) yields the Volterra competition model

$$\begin{aligned} \frac{dN_1}{dt} &= \epsilon_1 N_1 - \gamma_1(\alpha_1 N_1 + \alpha_2 N_2) \\ \frac{dN_2}{dt} &= \epsilon_2 N_2 - \gamma_2(\alpha_1 N_1 + \alpha_2 N_2) \end{aligned} \quad (4)$$

where

$$\gamma_i = q_i/p \; , \quad \epsilon_i = k_f \gamma_i - k_i > 0$$

3. Management with Proportionate Harvest

The Volterra competition model presented in equation (4) contains six parameters. It is easy to show, however, that the essential character of the response depends only upon the single non-dimensional parameter $r = \lambda_1/\lambda_2$ where $\lambda_i = \epsilon_i/\gamma_i$. There are three singular points or equilibrium states that the system can attain. If the equilibrium levels of population are defined as Q_1 and Q_2, these states are given by:

$$\begin{array}{lll} (a) & Q_1 = 0 & Q_2 = 0 \\ (b) & Q_1 = 0 & Q_2 = \epsilon_2/\alpha_2\gamma_2 \\ (c) & Q_1 = \epsilon_1/\alpha_1\gamma_1 & Q_2 = 0 \end{array} \qquad (5)$$

By normalising population size $X = N_1/Q_1$, $Y = N_2/Q_2$, and scaling time $\tau = \epsilon_1 t$ we obtain the following equations.

$$\frac{dX}{d\tau} = X[1 - X - Y/r]$$

$$q\frac{dY}{d\tau} = Y[1 - rX - Y] \qquad (6)$$

where

$$r = \lambda_1/\lambda_2,\ \lambda_i = \epsilon_i/\gamma_i$$

$$q = \epsilon_1/\epsilon_2$$

The equilibrium points associated with (6) are of course $(X^o=0,\ Y^o=0)$, $(X^o=0,\ Y^o=1)$ and $(X^o=1,\ Y^o=0)$. In order to examine the nature of these equilibria, we assume that X and Y experience small excursions x and y from their respective equilibrium levels. The linearized differential equations which arise from this excursion analysis are presented in equation (7) below.

$$\dot{\underline{z}} = A\underline{z}$$

where

$$\underline{z} = \begin{pmatrix} x \\ y \end{pmatrix} \qquad (7)$$

$$A = \begin{bmatrix} (1 - 2X^o - Y^o/r) & -X^o/r \\ -rY^o/q & (1 - 2Y^o - rX^o)/q \end{bmatrix}$$

Now, the roots of the characteristic equation $\det[sI - A] = 0$ determine the nature of the singular points. These roots are computed for each equilibrium state (X^o, Y^o) and are summarized in Table I.

equilib. point	roots of characteristic equation	nature of equilib. point
$X^o=0,\ Y^o=0$	$S_1=1, S_2=\frac{1}{q}$	unstable node
$X^o=0,\ Y^o=1$	$S_1=-\frac{1}{q}, S_2=(1-\frac{1}{r})$	stable node (r < 1) saddle point(r>1)
$X^o=1,\ Y^o=0$	$S_1=-1, S_2=\frac{(1-r)}{q}$	stable node (r>1) saddle point (r< 1)

Table I. Characterization of Equilibrium Points

These results demonstrate that the species with the largest value of $\lambda_i = \epsilon_i/\gamma_i$ will attain a stable equilibrium configuration at a finite, non-zero population level, while the weaker competitor is driven to extinction at the stable equilibrium configuration. This excursion variable analysis is born out globally in the phase portrait for the non-linear competition equations (see figure 1). Here it becomes evident that the stronger member drives out or replaces the weaker competitor.

In tne interest of preserving a balance between the two species allowing each to coexist with the other, one might choose a management policy in which harvest of the stronger species and/or replenishment of the weaker competitor is instituted; the intent here being to remove the competitive advantage of the stronger member of the system. Suppose that species Y is the stronger competitor and that the rates of harvest and replenishment are given by H and R respectively. Defining normalized, time scaled rates of $U = \alpha_1\gamma_1 R$ and $V = \alpha_2\gamma_2 H$ (where α_i and γ_i are the coefficients appearing in (4)) then the competition equations become:

$$\frac{dX}{d\tau} = X\,[1 - X - Y/r] + U$$

$$q\frac{dY}{d\tau} = Y[1 - rX - Y] - V \qquad (8)$$

Let us consider first the harvest strategy. Our first thought is to institute a program of proportionate harvesting, that is, a program in which a specified fraction of Y is removed. This is, perhaps, the simplest approach to take, since if a constant effort is made to harvest Y, then the yield will increase with larger numbers of species Y producing an approximately proportionate harvest. This is contrasted with the concept of an absolute harvest in which M members must be selected. In the absolute harvest the effort is adjusted to target the desired yield. In the proportionate harvest, then $V = f \cdot y$ and $U = 0$. The effect of such a strategy is to shift one of the singular points of the differential equation producing the following equilibrium configuration.

equilib. points	roots of characteristic equation	nature of equilib. point
$X^o=0, Y^o=0$	$S_1=1$ $S_2=(1-f)/q$	unstable node
$X^o=0, Y^o=(1-f)$	$S_1=-(1-f)/q$ $S_2=(r+f-1)/r$	stable node r + f < 1 saddle r+f>1
$X^o=1, Y^o=0$	$S_1=-1$ $S_2=(1-r-f)/q$	saddle r+f< 1 stable node r + f > 1

Table II. The Effect of Proportionate Harvesting on Equilibria (f< 1)

If the harvest fraction is sufficiently large, the originally weaker species will dominate the ecology. If this management policy is continued indefinitely, the harvested species, once the dominant competitor, will be driven toward extinction. If one desires a scheme whereby both species can co-exist, it is possible to institute a program in which a period of harvest is followed by a period of "natural growth". This strategy would render alternating advantages to the two species producing (if properly implemented) a limit cycle or closed periodic solution in the phase plane. Since neither species is permitted to dominate the ecology for a sufficiently long period of time, both can coexist.

4. Management with Absolute Harvest and Replacement

An alternate procedure for controlling the growth in this ecological system is to impose an absolute harvest. Contrasted to the proportionate policy, the absolute harvest involves the setting of a target harvest level; the harvesting of the stronger species is continued until this target is achieved. In a similar fashion we could consider a constant replenishment program for the weaker species. If U and V are the constant levels of replacement and harvest, the equations which describe the growth within the competitive system are

$$\frac{dX}{d\tau} = f(X, Y, U)$$
$$q\,\frac{dY}{d\tau} = g(X, Y, V) \tag{9}$$

where

$$f(X, Y, U) = X[1 - X - Y/r] + U$$
$$g(X, Y, V) = Y[1 - rX - Y] - V$$

Setting f and g to zero yields a pair of simultaneous equations in X and Y; for any level of harvest V and replacement U these equations can be solved to obtain the equilibrium points. Graphically, one can interpret f=0 and g=0 as families of curves parameterized in U and V respectively. These curves are illustrated in figure 2. The intersection of any f=0 curve with another g=0 curve yield these equilibria. A few equilibrium points are illustrated in the figure.

Once the equilibrium point is established, we must determine the character of the equilibrium point - does it represent a stable or an unstable configuration? We proceed to obtain the characteristic equation from the linearized form of the describing equations

$$\frac{dx}{d\tau} = \frac{\partial f}{\partial X}x + \frac{\partial f}{\partial Y}y$$
$$q\frac{dy}{d\tau} = \frac{\partial g}{\partial X}x + \frac{\partial g}{\partial Y}y \tag{10}$$

obtaining

$$\det[sI - A] = s^2 + as + b = 0$$

where

$$A = \begin{bmatrix} \partial f/\partial X & \partial f/\partial Y \\ \partial g/\partial X & \partial g/\partial Y \end{bmatrix} \quad ; \; a = -\left[\frac{\partial f}{\partial X} + \frac{1}{q}\frac{\partial g}{\partial Y}\right]$$
$$b = \frac{1}{q}\frac{\partial f}{\partial Y}\frac{\partial g}{\partial Y}[S_g - S_f]. \tag{11}$$

Now S_g and S_f are slopes of the curves g=0 and f=0 at the equilibrium point. Consider the illustration in figure 3. At equilibrium point I the geometry of the curves is such that the partial derivatives of both f and g with respect to each coordinate are negative, thus $a > 0$ and since $S_g > S_f$ the coefficient $b > 0$. The nature of the singular point depends upon the coefficients a and b;[5] this dependence is illustrated in figure 4. We know immediately that the equilibrium point must be stable; if in addition it is possible to demonstrate that $a^2 > 4b$ then we would know that the equilibrium configuration would be a stable node. Using the fact that $S_f = -(\partial f/\partial X)/(\partial f/\partial Y)$ and $S_g = -(\partial g/\partial X)/(\partial g/\partial Y)$ we can write this inequality as

$$\left(\frac{\partial f}{\partial X} - \frac{1}{q}\frac{\partial g}{\partial Y}\right)^2 > -\frac{4}{q}\frac{\partial f}{\partial Y}\frac{\partial g}{\partial X}. \tag{12}$$

Since $\partial f/\partial Y$ and $\partial g/\partial X$ have the same sign $a^2 > 4b$ and from figure 4 we see that the singular point is a stable node. Similar reasoning leads to the conclusion that for equilibrium point II $b < 0$. Again figure 4 can be used to establish this to be a saddle point. Both species can coexist at the stable equilibrium point; the motion of this system toward the equilibrium point is illustrated in the phase portrait of figure 5.

It is interesting to consider the special case in which the replacement rate $U = 0$ while the harvest rate $V > 0$. Under these conditions no such stable equilibrium point exists such that both $X > 0$ and $Y > 0$. Thus an absolute harvest policy with no replacement will not achieve our stated objectives failing to produce a balance within the system (see figure 5). The compliment of this strategy in which replacement is instituted without harvest does produce a desired stable equilibrium point; this conclusion can be reached using the geometric arguments presented above.

5. Summary

In the unmanaged Volterra competition system, the stronger species will replace the weaker competitor. Proportionate harvest alters the balance within the ecology, and can effect a competitive advantage to the originally weaker species. A continuous application of such a management strategy merely shifts the competitive advantage; again the system is driven toward dominance by a single member. Absolute harvest alone does not produce a stable equilibrium configuration in which both species can coexist. A combined policy which implements both an absolute harvest of the stronger member and the replacement of the weaker competitor can induce a balance within the system.

The design of such a strategy is based upon the control curves presented in figure 2. Although these curves were developed for the Volterra competition equations, they can be modified if any of the assumptions of linearity presented in the model development are deemed inappropriate. Levels of harvest and replacement are then selected such that $X > Y_{min}$ and $Y > Y_{min}$ at the equilibrium .

6. References

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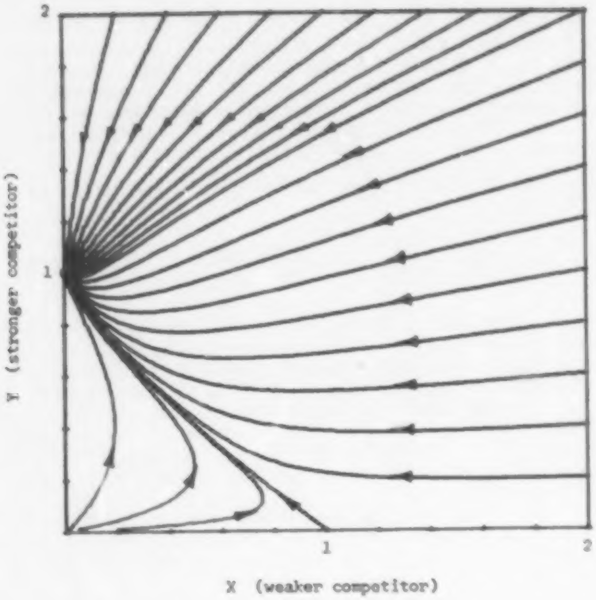

Figure 1. Unmanaged Competition

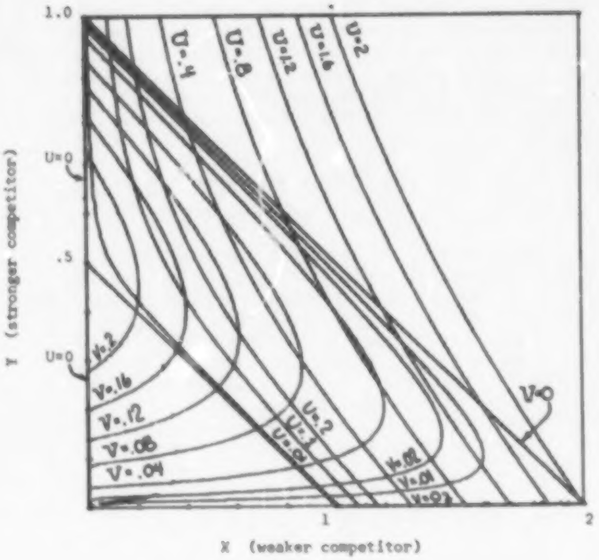

Figure 2. Control Curves for Selecting Harvest and Replacement Rates

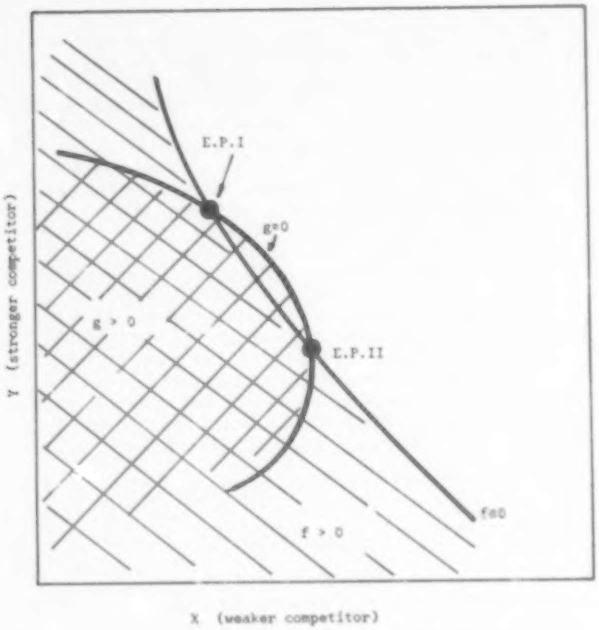
E.P.I
g=0
g > 0
E.P.II
f=0
f > 0
Y (stronger competitor)
X (weaker competitor)

Figure 3. Representative Control Curves

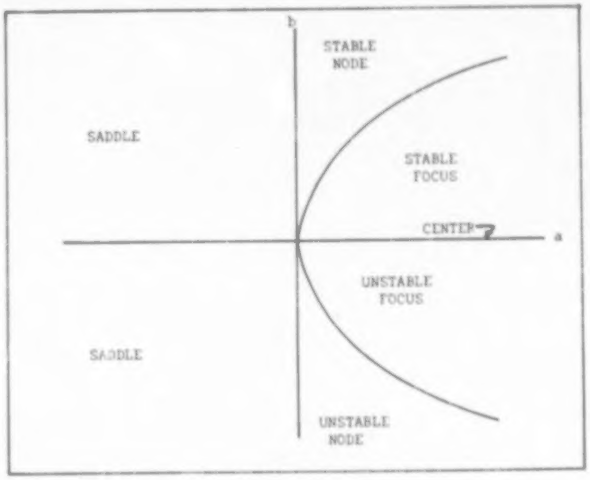
b
STABLE NODE
SADDLE
STABLE FOCUS
CENTER
a
UNSTABLE FOCUS
SADDLE
UNSTABLE NODE

Figure 4. Nature of Roots of Characteristic Equation

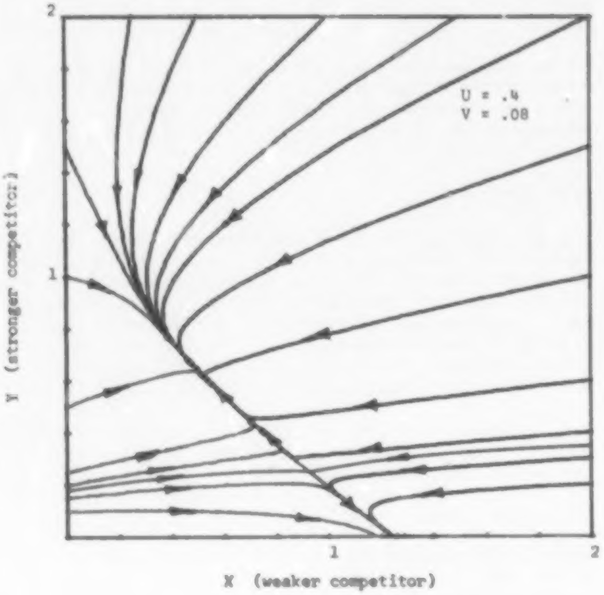

Figure 5. Competition with both Harvest and Replenishment

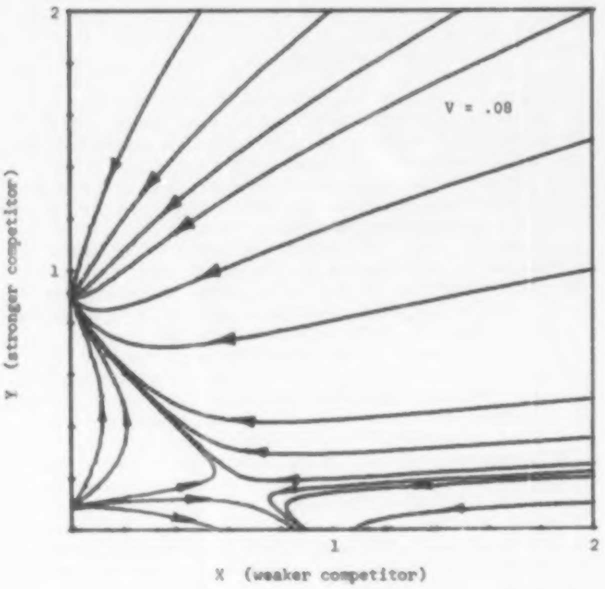

Figure 6. Competition with Harvest Management

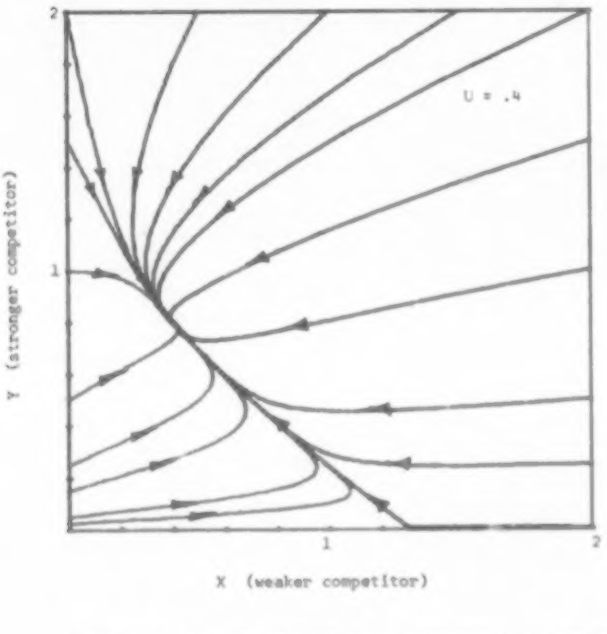

Figure 7. Competition with Replacement Management

PLANNING IMPLICATIONS OF DISSOLVED OXYGEN DEPLETION IN THE WILLAMETTE RIVER, OREGON

David A. Rickert, Walter G. Hines, and Stuart W. McKenzie
U.S. Geological Survey
Portland, Oregon

ABSTRACT

Basinwide secondary treatment of municipal and industrial wastewaters has resulted in a dramatic increase of summertime dissolved-oxygen (DO) concentrations in the Willamette River. Rates of carbonaceous decay (k_1) are very low (0.03 to 0.06/day), and point-source BOD loading now accounts for less than one-third of the satisfied oxygen demand. Nitrification is now the dominant DO sink. DO concentrations met the state standards in all reaches of the Willamette during the low-flow period of 1974. Mathematical modeling shows that low-flow augmentation from storage reservoirs was largely responsible for the standards being met. Future achievement of DO standards will require continued low-flow augmentation in addition to pollution control. Summertime flows above 6000 ft^3/s will be needed even with increased treatment removals of oxygen depleting materials. The greatest immediate incremental improvement in DO can be made through reduction in point-source ammonia loading. The pros and cons of upgrading treatment efficiencies for BOD removal would best be determined after ammonia loadings have been reduced to reasonable levels and the possibility of controlling a benthal-oxygen demand in Portland Harbor has been fully assessed.

(KEY TERMS: river-quality planning; dissolved-oxygen standards; dissolved-oxygen modeling; biochemical-oxygen demand; nitrification; low-flow augmentation.)

INTRODUCTION

Historically, dissolved-oxygen (DO) depletion has been the critical water-quality problem in the Willamette River. During summer low-flow periods, DO concentrations of zero were sometimes observed in Portland Harbor (see figure 1), and for years, low DO levels inhibited the fall migration of salmon from the Columbia River.[1]

In recent years, summer DO levels have increased dramatically. The improvement has resulted primarily from the basinwide advent of secondary wastewater treatment, coupled with streamflow augmentation from storage reservoirs. With an average annual flow of 35,000 ft^3/s, the Willamette is now the largest river in the United States on which all known point sources of wastewaters receive secondary treatment. The Willamette thus offers a unique opportunity to document the impacts of secondary treatment on a large river and also to predict the amount of further improvement likely to result from different alternatives of river-basin management.

PHYSICAL SETTING

Willamette River Basin

The Willamette River basin, a watershed of almost 11,500 sq mi (figure 1), is located in northwestern Oregon between the Cascade and Coast ranges. Within the basin are the state's three largest cities, Portland, Salem, and Eugene, and approximately 1.4 million people, representing 70 percent of the state's population (1970 census). The Willamette River basin supports an important timber, agricultural, industrial, and recreational economy and also extensive fish and wildlife habitats.

The basin is roughly rectangular, with a north-south dimension of about 150 mi and an east-west width of 75 mi. Elevations range from less than 10 ft near the mouth of the Willamette River to 450 ft on the valley floor near Eugene and to more than 10,000 ft in the Cascade Range. Average annual precipitation in the basin is 63 inches.

Hydrology

Channel Morphology.--The Willamette River main stem forms at the confluence of its Coast and Middle forks south of Eugene and flows northward for 187 mi through the Willamette Valley floor. The river is composed of three morphological reaches (figure 1 and table 1). Each reach has a unique hydraulic regime and, therefore, different velocities, sediment-transport characteristics, and patterns of biological activity.

The Upstream Reach, stretching from above Eugene to near Newberg, is shallow and fast-moving. The riverbed is composed largely of cobbles and gravel which provide ample opportunity for attachment of periphytic biological growths. During the summer low-flow period, mean velocity in this reach is about seven times that observed in the Newberg Pool and 18 times greater than in the Tidal Reach. Morphologically, this section of the river is an "eroding" reach.

Between a point just above Newberg and the Willamette Falls is a deep, slow-moving reach known as the Newberg Pool. Hydraulically, the Pool can be characterized as a large stilling basin behind a weir (Willamette Falls). Travel time in this 25.5-mi reach is relatively long during low-flow conditions. Morphologically, the Pool is a depositional reach.

The lower 26.5 mi of the river is affected by tides (nonsaline water) transmitted from the Pacific Ocean via the Columbia River and, during April to July, by backwater from the Columbia. The Tidal Reach is dredged to maintain a 40-ft-deep navigation channel up to river mile (RM) 14. During low flows, net downstream movement in the Tidal Reach is slow, but tidal flow reversals can cause large instantaneous changes in velocity. Low-flow hydraulics are most complex in the lower 10 mi where, depending on hourly changes in tidal conditions, Willamette River water may move downstream or Columbia River water upstream. Owing to morphological characteristics and the hydraulic conditions, the subreach below RM 10 is the primary depositional area of the Willamette River.

Flow.--Most of the flow in the Willamette occurs in the November to March period as a result of persistent winter rainstorms and spring snowmelt. Each summer there is a naturally occurring low-flow period, the timing, duration, and magnitude of which are now largely controlled by reservoir releases. Since 1954, when large-scale reservoir regulation began, discharge during the low-flow period of July-August has been maintained at a minimum of about 6000 ft^3/s (Salem gage) by reservoir augmentation. In comparison, for the unusually dry year of 1973, the calculated (from a deterministic model) naturally occurring low flow for this period would have been 3260 ft^3/s. The summertime flow releases are made for purposes other than river-quality enhancement, but, as subsequently described, the augmentation has a profound impact on the DO regime.

Temperature.--Water temperatures in the Willamette River and in all tributaries reach a maximum during the annual July-August low-flow period. Temperatures during July average about 20° C in the Newberg Pool and about 22° C in the Tidal Reach; these are controlled primarily by ambient air temperatures.

DATA PROGRAM

Review of existing data indicated that an appreciable DO deficit occurs in the Willamette only below RM 86 and during the yearly low-flow period of July through August. The DO-data-collection program was developed to formulate a mathematical model for simulating conditions below RM 86 for the critical summer period. Emphasis was placed on direct intensive measurement of waste loads and model coefficients to avoid reliance on published values, engineering estimates, and the development of model coefficients through computerized curve fitting (optimization). Details of sampling approaches and analytical techniques are reported in other papers.[2,3,4]

DISSOLVED-OXYGEN REGIME

Dissolved-Oxygen Profiles

Basinwide secondary treatment has had a profound impact on the major deoxygenation processes and consequently on the DO regime of the Willamette River. During the summer low-flow period of 1974, average daily DO concentrations met state standards for all reaches of the river at flow conditions between 6500 and 7000 ft^3/s and water temperatures between 22° and 25° C.

Figure 2 compares the 1973 DO profile of the river below RM 86 to historic conditions. In 1956, there was a DO-concentration "plateau" between Salem and Newberg, followed by a sharp decrease in DO through the Newberg Pool. These conditions were consistent with large loadings of carbonaceous biochemical oxygen demand (BOD) in the vicinity of Salem, a rapid travel time between Salem and Newberg, and a large amount of carbonaceous deoxygenation in the slow-flowing Newberg Pool.

The 1959 data show an increase in DO concentration below Willamette Falls and a sharp decrease in DO through the Tidal Reach. These observations were consistent with known reaeration at the falls, inflow of cool high-DO water from the Clackamas River, and the decay of carbonaceous wastes which entered the river just below the falls and throughout Portland Harbor.

The 1973 profile shows a rapid decrease of DO from RM 86 to Newberg, a DO "plateau" in the Newberg Pool, a DO increase over Willamette Falls, a gradual decline in DO between RM's 24 and 13, a sharp decrease in DO between RM's 13 and 5, and recovery of DO below RM 5. The DO decrease between RM 86 and Newberg contrasts with a "plateau" in 1956 and results from nitrification that did not occur at the earlier date. The 1973 DO "plateau" in the Newberg Pool indicates that carbonaceous deoxygenation is now occurring at a rate slow enough to be balanced by DO inputs from atmospheric reaeration. The DO decrease between RM's 24 and 13 is consistent with measured river loads of ultimate BOD (BOD$_{ult}$), but the sharp decrease between RM's 13 and 5 cannot be accounted for by known sources of BOD. (See section entitled "Benthal-Oxygen Demand.") The DO profile of the Willamette during July-August 1974 was essentially the same as that presented in figure 2 for 1973.

Nitrification

During the summers of 1973 and 1974, nitrification was the dominant control on DO in the shallow, swift-flowing subreach between RM's 85 and 55. Examination of historical data indicates that this reach began to receive appreciable ammonia loading from a pulpmill in 1956. Dissolved-oxygen data from the 1950's and 1960's are sketchy, but suggest that nitrification did not become a significant oxygen sink until the advent of secondary treatment at pulp and paper mills. Secondary treatment incurred the use of ammonium hydroxide for neutralizing wastewaters prior to treatment, and resulted in continuous discharge of effluents to the Willamette rather than the previously used program of summer lagooning and winter discharging.

Figure 3 shows the average instream concentrations of ammonia, nitrite, and nitrate nitrogen from RM 120 to 7 for August 12-14, 1974. The curves reflect a prominent ammonia source near RM 116 and rapid instream oxidation of ammonia to nitrite and nitrate downstream to RM 86. During the study period, the subreach below RM 86 received about 5800 lb/d ammonia nitrogen from upstream sources, 16,200 lb/d from an ammonia-base pulp and paper mill at RM 85, and about 1700 lb/d from a municipal sewage plant at RM 78. The instream data show a rapid conversion of the ammonia to nitrite and nitrate between RM's 85 and 55. The deep, relatively slow-moving Newberg Pool begins at RM 52 and, although residual ammonia entered this reach, no further nitrification could be detected from nitrogen-species analysis.

The occurrence of nitrification in a shallow, surface-active reach and the contrasting absence in a deep, slow-moving reach is consistent with a recent hypothesis proposed by Tuffey, Hunter, and Matulewich.[5] According to the hypothesis, nitrification in shallow, swift-flowing reaches would occur by virtue of an attached, rather than a suspended population of nitrifying organisms. To test the hypothesis, enumerations of nitrifying bacteria were made on water samples and on biological slimes scraped from rocks. *Nitrosomonas* concentrations were <1 most probable number (MPN)/ml in all water samples from throughout the river. In slimes, *Nitrosomonas* concentrations were <1 MPN/mg above RM 86 and 1-4 MPN/mg in samples collected between RM's 85 and 55 (the active zone of nitrification). The Newberg Pool is a deep depositional reach and few rocks are available for attachment. In comparison, *Nitrobacter* concentrations in the zone of nitrification ranged from <1 to 4 MPN/ml in water samples and from 6-50 MPN/mg in slimes. The bacteriological data thus support the hypothesis that nitrification occurred in slimes attached to rocks rather than in flowing water.

Based on observed river concentrations of nitrate (figure 3), an in-river rate of nitrification was calculated for the affected subreach. Assuming first-order decay, the rate, k_n ($\log_{10}$), was about 0.7/d. Applying this rate to the measured loadings of ammonia indicates that, for the August 12-14 period, nitrification removed about 55,000 lb/d DO from the 30-mi subreach. This satisfied demand was responsible for most of the decrease observed in DO concentration (figure 2).

Carbonaceous Deoxygenation

Present-day (1974) BOD-loading patterns and rates of exertion contrast sharply with those observed during the mid-1950's.

BOD Loading.--During the dry-weather period of 1954, the estimated point-source loading of BOD_{ult} to the Willamette River was approximately 350,000 lb/d. This total included chemical demands resulting from sulfite wastes, soluble and suspended carbonaceous demands from pulp and paper mills, and the carbonaceous demands of raw sewage and primary effluents.

In contrast, the point-source BOD_{ult} loading during August 1974 was about 92,000 lb/d (table 2). The decrease resulted from secondary treatment of all carbonaceous wastes, chemical recovery of sulfite wastes, and the routing of sewage effluents from metropolitan Portland into the Columbia River instead of the Willamette.

During the 1974 low-flow period, nonpoint sources contributed about 77,000 lb/d BOD_{ult} to the Willamette, or about 46 percent of the total basin-wide loading (table 2). Because of the design of the nonpoint-sampling program, it appears that almost all of the estimated loading from diffuse sources represents natural background demand from essentially pristine streams. Thus, only about one-half the observed total BOD_{ult} loading to the Willamette River is potentially amenable to removal by future pollution-control programs.

Concentrations and Rates.--During the low-flow period of 1954, five-day BOD's (BOD_5) in the Willamette River varied from about 1.0 mg/l at sites far removed from waste inputs to about 2.5 mg/l below large waste outfalls. During 1974, measured BOD_5 concentrations were about 1.0 mg/l throughout the river. The apparent anomaly of the comparative concentrations arises from marked differences between 1954 and 1974 in the river rates of deoxygenation (k_1). The value throughout the river in 1954 was probably 0.1/d ($\log_{10}$) or greater.[6] The measured k_1's in 1974 were clustered around 0.04/d. Thus in 1954, a minimum of about 68 percent of BOD_{ult} was exerted in five days, whereas in 1974 the comparative value was 39 percent (see Velz for discussion of BOD exertion).[7] This comparison underscores the need for determining k_1 values and BOD_{ult} (rather than BOD_5 alone) as a basis for accurately modeling DO under conditions of secondary treatment.

The in-river concentrations of BOD_{ult} during 1973 and 1974 averaged about 2.5 mg/l.

Benthal-Oxygen Demand

During 1970, benthal respirometer studies (written communication, John Sainsbury, 1970) of the Willamette documented a benthal-oxygen demand of 27,000 to 54,000 lb/d in the subreach between RM's 13 and 7. The river at that time still received some raw sewage in the form of combined sewer overflows and a moderate loading of settleable solids from pulp and paper mills. Because these sources of solids are now largely controlled, it was anticipated that the benthal demand would be greatly reduced by 1973. However, during preliminary calibration of our model, predicted DO concentrations between RM's 13 and 5 were higher than those measured in the river, whereas predicted BOD_{ult} concentrations were considerably lower. Refined modeling tests suggested an unaccounted-for oxygen demand of about 27,000 lb/d in the subreach.

DO Modeling

The model chosen for the study was the one developed and used for more than 30 years by C. J. Velz. The basic model, described in detail in *Applied Stream Sanitation*,[7] is applicable to conditions of steady (invariable), nonuniform (changing cross-sectional geometry), plug (nondispersive) flow. The computer program as formulated for the present study is called the WIRQAS (Willamette Intensive River Quality Assessment Study) model.

The model was calibrated against 1974 streamflow and temperature conditions and verified against the slightly lower flow and higher temperature conditions of 1973. For conditions representing 1974 summer low, the model indicates that an oxygen demand of 164,000 lb/d was satisfied between RM's 86 and 5. Of the total, about 22 percent resulted from background carbonaceous-oxygen demand, 28 percent from point-source carbonaceous demand, 34 percent from point-source ammonia, and 16 percent from the unaccounted-for demand in Portland Harbor.

PLANNING IMPLICATIONS

As an aid to river-quality planning, the WIRQAS model has been used to test management alternatives concerning (1) BOD loading, (2) ammonia loading, (3) low-flow augmentation, and (4) the effects of possible removal or reduction of the benthal-oxygen demand. This section describes the major implications of tested alternatives by comparing measured DO profiles with profiles generated by the verified model. A fact the reader should bear in mind in examining the following illustrations (figures 4-8) is that, for ease of presentation, the DO profiles are plotted as a function of river location. Thus the slopes of curves in specific subreaches do not represent the actual rates at which oxygen is added to or lost from the river. For example, the profiles in figures 4-8 suggest a rapid rate of oxygen depletion below Willamette Falls. Actually, the steepness of the curves is caused by the slow time-of-travel in the Tidal Reach (see table 1) rather than by an accelerated rate of oxygen depletion.

BOD Loading

The effect of BOD loading on summertime DO is reflected in figure 4. The curve labeled 100 percent represents the average DO profile of the river at the flow, water temperatures, ammonia loading, and BOD loading actually measured during the low-flow, steady-state period of mid-August 1974. The upper and lower curves represent the predicted DO profiles at 50 percent and 200 percent of the measured point-source BOD loading with all other variables held constant at observed levels. These curves are calculated on the basis that all point-source BOD receives secondary treatment and decays at rates of 0.06/d above RM 55 and 0.03/d below this point.

The upper curve in figure 4 indicates that only a slight improvement in DO can be obtained by a 50 percent decrease of BOD loading from each point source in the basin. The predicted increase in DO would be <5 percent of saturation at the bottom of the Newberg Pool (RM 28) and 5 percent at RM 5, the low DO point in the river.

In contrast, a doubling of BOD loading from each point source would depress DO by 5 percent of saturation at RM 28 and by 10 percent at RM 5. This decrease in DO would cause violation of the state DO standard in the subreach between RM's 62 and 50.

Figure 5 compares the DO profile observed in mid-August 1974 with the predicted profile assuming a BOD_5 standard of 10 mg/l for all municipal wastewater effluents. Such a standard, attainable by high-level secondary treatment, is presently being considered by Oregon and several other states throughout the country. Application of the 10 mg/l standard in the Willamette River basin would decrease municipal summertime loading of BOD_{ult} from 37,600 lb/d to 17,400 lb/d. The largest individual decrease would be about 7000 lb/d at Salem (RM 78). The modeling results (figure 5) indicate that, over the investigated reaches, the reduced loading would have no effect on river DO. The lack of an effect stems from (1) the small reduction attainable in total loading of BOD_{ult} (about 12 percent; see table 2), (2) the low rate at which BOD_{ult} is exerted in the river, and (3) the locations within the basin of the largest municipal wastewater treatment plants.[4]

Ammonia Loading

Figure 6 illustrates the effect of ammonia loading on summertime DO in the Willamette. Compared to the observed DO profile (the 100 percent curve), a 50 percent reduction in ammonia-nitrogen loading from each point source would increase the DO by 7 percent of saturation near the bottom of the Upstream Reach (RM 60), by 5 percent at RM 28, and by <5 percent at RM 5. In contrast, a doubling of ammonia-nitrogen loading in each point source would decrease the DO by 13 percent at RM 60, by 11 percent at RM 28, and by 7 percent at RM 5. These results illustrate two important points. First, ammonia loading has its greatest effect on DO in the active zone of nitrification between RM's 85 and 55. Thereafter, measurable nitrification ceases to occur and the upstream effects of the process are gradually diminished by atmospheric reaeration. Second, comparison of figures 4 and 6 indicates that point-source ammonia loading has a greater influence on Willamette River DO than point-source BOD loading. At the observed relative point-source loadings (43,000 lb/d ammonia-nitrogen; 92,000 lb/d BOD_{ult}), this occurs primarily as a result of (1) the greater oxygen demand per unit weight of ammonia as compared to the organic matter in secondary effluents, and (2) the much greater rate at which ammonia is oxidized ($k_1 = 0.03$ to 0.06/d; $k_n = 0.7$/d).

The upper curve in figure 6 shows the impact of applying a standard of 10 mg/l ammonia-nitrogen to all municipal and industrial effluents.

Most of the ammonia that enters the Willamette below RM 86 is discharged from a large pulp and paper mill at RM 85 (see "Nitrification"). Control of ammonia from this one source would greatly reduce the impact of nitrification on the DO regime of the river.

Low-Flow Augmentation

The effect of flow augmentation on DO is illustrated in figure 7. The observed flow at Salem during mid-August 1974 was 6760 ft^3/s. For comparison, computed DO profiles are presented for Salem flows of 9000, 5000, and 3260 ft^3/s. The latter value is near the lowest minimum monthly average flow ever observed for July under natural (nonaugmented) conditions.[6] As previously noted, predictions from a deterministic model indicate this flow would have occurred during July of the unusually dry year of 1973.

The impact of flow augmentation is marked. At a flow of 3260 ft^3/s, the 1974 BOD and ammonia-nitrogen loadings would cause violation of state DO standards by a wide margin at most locations. The predicted DO saturation levels at 3260 ft^3/s are nearly 30 percent less than the observed values (6760 ft^3/s) at RM's 60, 28, and 5. At a flow of 5000 ft^3/s, the state DO standard would have been violated between RM's 67 and 50 and just have been met in the Newberg Pool.

In contrast to the marked decrease predicted in DO at decreased flows, an increase to 9000 ft^3/s would cause a relatively small improvement in saturation percentages. The effects of augmentation on Willamette River DO result from a complex interaction of flow with (1) the loading and rate of BOD exertion, (2) ammonia loading and the rate of nitrification, (3) time of travel, and (4) atmospheric reaeration. The most significant interactions at different levels of flow have not been delineated, but it appears under the combined conditions observed in 1974 that flow augmentation to discharges above 7000 ft^3/s would provide little incremental increase in DO concentrations. However, under future conditions, flows in excess of 7000 ft^3/s might be a desirable alternative to expensive, energy-consuming advanced-waste treatment processes.

Figure 8 illustrates the combined effects of nitrification and flow augmentation. Curve B is the average DO profile observed during the steady, low-flow period of July-August 1973. Curve D is the predicted DO profile at a flow of 3260 ft^3/s and the observed ammonia loading. In comparing curves B and D, note that without augmentation, the state DO standards would have been violated at most points in the river. Curves A and C represent predicted DO profiles at the same two flows, but with ammonia-nitrogen loading reduced to 10 mg/l in all point-source discharges. With such an effluent limitation, the DO profile predicted at 6000 ft^3/s is considerably above the observed profile (curve B) throughout most of the river. However, curve C portrays the most important finding for 1973 conditions. Even with basinwide secondary treatment and a reasonable limitation on ammonia loading, low-flow augmentation would be necessary to achieve DO standards in the Newberg Pool and the Tidal Reach.

Benthal-Oxygen Demand

As previously noted, the WIRQAS model indicates the presence of an unaccounted-for oxygen demand of 27,000 lb/d between RM's 13 and 7. Field investigations suggest that most of the demand is benthal in origin, but the exact causes are unknown. Possible factors that may either cause or affect the oxygen demand include:

1. Unknown sources of raw sewage.
2. Combined-sewer overflows.
3. Urban storm runoff.
4. Bilge water and refuse from ships.
5. A net oxygen loss caused by algal respiration exceeding algal production owing to limited light penetration of the water column.
6. A turbid, high-oxygen demanding, estuarine-like "null zone" resulting from tidally influenced hydraulic conditions.
7. Sedimentation and decomposition of natural organics such as leaves and algae.

These possibilities are presently the focus of further study. Hopefully, all or at least part of the demand can be related to controllable sources. If so, management control of these sources will provide a means for improving summertime DO by up to 8 percent of saturation at RM 5.

SUMMARY AND CONCLUSIONS

Future achievement of DO standards in the Willamette River will require continued low-flow augmentation in addition to pollution control. Minimum flows of 6000 ft^3/s (Salem gage) are presently (1974) needed to meet the standards at existing BOD and ammonia loadings and with the occurrence of an unidentified (probably benthal) oxygen demand in Portland Harbor. As basin development continues, it is likely that summertime flows above 6000 ft^3/s will be needed even with increased treatment removal of oxygen-depleting materials.

Point-source loading of ammonia is presently the major cause of oxygen depletion below RM 86. Because most of the ammonia comes from one source, reduction of ammonia loading offers a relatively simple alternative for achieving a large improvement in summertime DO.

Removal or partial reduction of the oxygen demand in Portland Harbor would improve the summer DO concentrations between RM's 10 and 5. However, the feasibility of reducing the demand is yet to be determined.

BOD loading from municipal wastewater treatment plants presently exerts a relatively small impact on DO. Increased efficiency of BOD removal at the largest municipal plants and at selected industrial plants might be desirable in the future. The benefits to be gained from this alternative would best be determined after ammonia loadings have been reduced to reasonable levels and the possibility of controlling the suspected benthal demand has been fully assessed.

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TABLE 1. Physical Characteristics of the Main Stem Willamette River (for discharge at Salem = 6000 ft^3/s).

Reach	Length, miles	Approximate bed slope, ft/mile	Bed material	Representative midchannel water depth, ft	Average velocity, ft/s	Approximate travel time in reach, days
1 Tidal	26.5	0.1	Clay, sand, and gravel	40	0.16	10
2 Newberg Pool	25.5	.12	do	25	.40	3.9
3 Upstream	135	2.8	Cobbles and gravel	7	2.9	2.8

TABLE 2. Dry-Weather 1974 Ultimate BOD Loading, Willamette River, Oregon

Sources	Loading, lbs/day	Percent
Nonpoint	77,100	46
Point		
Municipal	37,600	22
Industrial	54,400	32
Total:	169,100	100

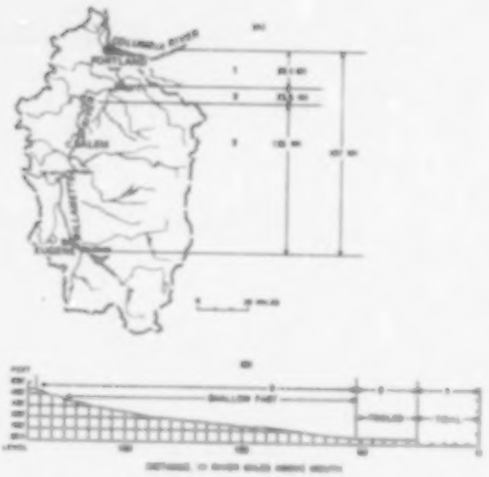
COLUMBIA RIVER
PORTLAND
SALEM
EUGENE
WILLAMETTE
1
2
3
SHALLOW FAST
POOLED
TIDAL
FEET
DISTANCE, IN RIVER MILES ABOVE MOUTH

Figure 1. -- Map and profile representing the Willamette River, Oreg., (A) distinctive morphologic reaches, (B) elevation profile.

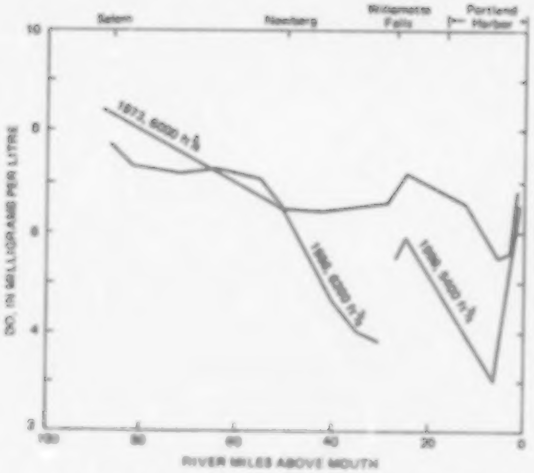

Figure 2. -- Comparison of 1973 and historical DO profiles in the Willamette River for steady, low flow conditions.

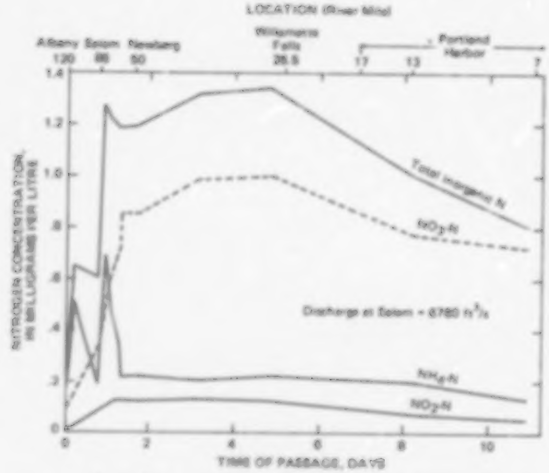

Figure 3. -- Inorganic nitrogen concentrations in the Willamette River during mid-August 1974.

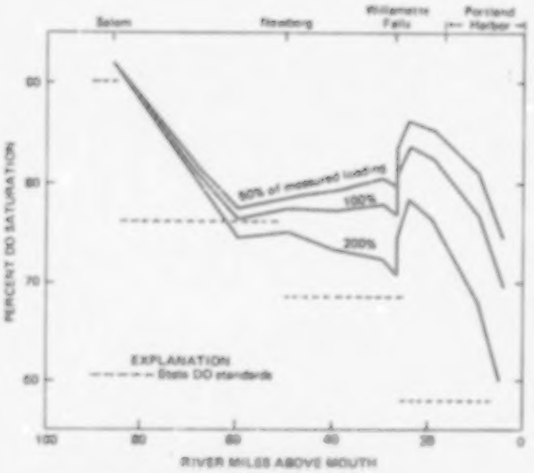

Figure 4. -- DO profiles for selected percentages of the measured point-source BOD loading during mid-August 1974. Flow and ammonia loading held constant at observed levels.

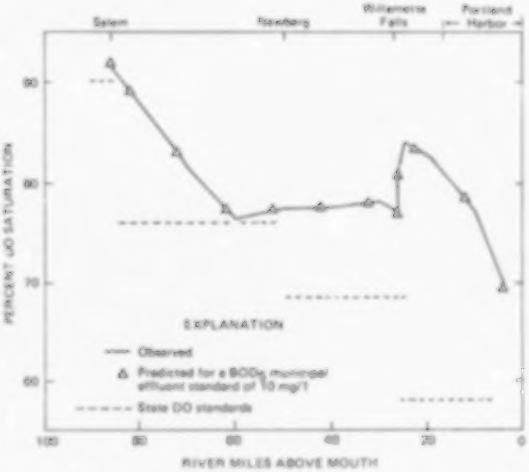

Figure 5 — DO profiles: observed during mid-August 1974 and predicted for a BOD$_5$ municipal effluent standard of 10 mg/1. Flow and ammonia loading held constant at observed levels.

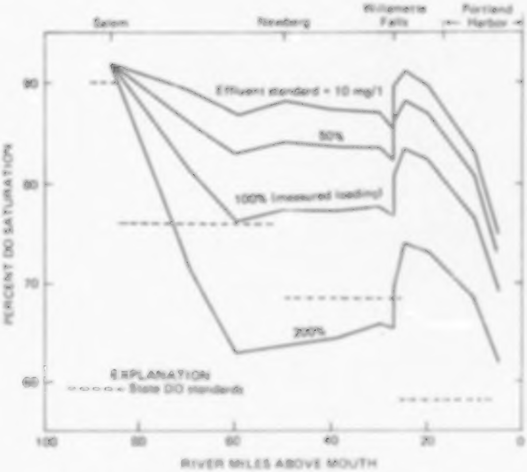

Figure 6 — DO profiles for an effluent standard of 10 mg/1 NH$_4$-N and for selected percentages of the measured point-source ammonia loading during mid-August 1974. Flow and BOD loading held constant at observed levels.

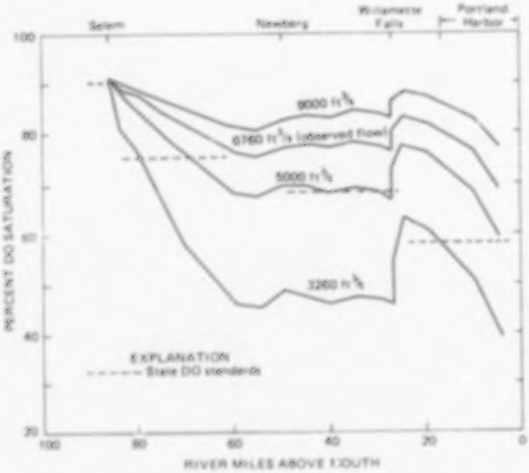

Figure 7 — DO profiles for selected flows with BOD and ammonia loadings held constant at levels measured during mid-August 1974. Observed flow was about 6,760 ft^3/s.

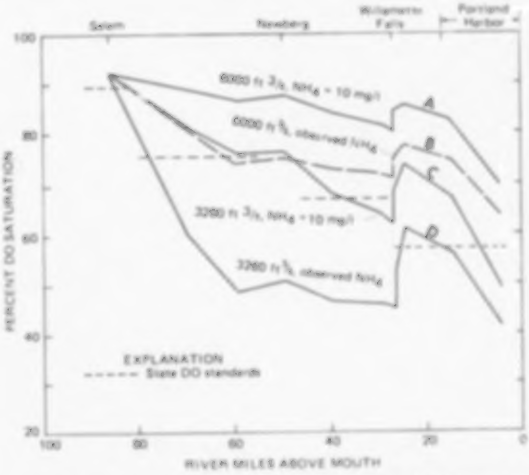

Figure 8. — DO profiles for selected conditions of flow and ammonia loading. BOD loading held constant at levels observed during July-August, 1973. Curves A, C and D are predicted; curve B is observed.

URBANIZATION AND FLOODING - AN EXAMPLE

Robert P. Shubinski, Vice President and William N. Fitch, Principal Engineer
Water Resources Engineers, Inc.
Springfield, Virginia

Summary

The Four Mile Run watershed in Northern Virginia is a classical example of the development of flood problems with urbanization. The Corps of Engineers has planned $29,000,000 in channel improvements to alleviate the problem, but the Congress, concerned that future development in the basin will create the problem again, required that a land management program be developed. The selected approach to land management is designed to determine effective structural and nonstructural methods of flood abatement. Emphasis is on the nonstructural. The technical portions of the program rely on two stormwater models. The models are STORM, a Corps model which is useful as a screening tool, and SWMM, a more detailed model sponsored by EPA. The paper describes the application of these models, using historic and design hydrology, to determine the plans and policies for further basin development.

Introduction

This paper describes the application of two complementary stormwater models to an urbanizing watershed. The first model, STORM (Storage, Treatment, Overflow, Runoff Model),[1] is a simple model based on the rational method. It was used to develop a statistical analysis of the basin's hydrology, thereby defining the design storm. The sophisticated model, WREM (Water Resources Engineers Model),[2] was then applied, using the design hydrology developed in STORM, to determine the response of the watershed to various control alternatives. Later, in work now underway, these results will be used to assign design shares for future development to each of the political subdivisions in the basin.

The Overview Model, STORM

The Four Mile Run Basin, located in Northern Virginia, has a total watershed area of 19.5 square miles. Figure 1 is a map of the basin. There are five major tributaries, all of which have steep slopes and in general have rapid and very peaked runoff characteristics. The base flow of Four Mile Run, for the purposes of this study defined as the dry weather flow, varies from 3 to 7 cfs. This discharge is insignificant compared to peak discharge rates for flooding events and was therefore not included in the flood flow analysis.

Three types of hydrologic data were prepared as input to STORM: areal and temporal distribution of rainfall, stream flood stage and evaporation rate. Rainfall distribution data were analyzed to identify significant long term trends in the major storm events and the type of storm which creates major floods, and to define reliable isohyetal patterns for the major storm events. Data for this study were taken from recording and nonrecording rainfall gages operated in 60 different locations in and around the watershed by the United States Geological Survey (USGS), the National Weather Service (NWS), and Arlington and Fairfax Counties.

Temporal data indicated that higher intensity rainfalls occurred during thunderstorms rather than during hurricanes or slow-moving storms and the time at which peak intensities occur for different stations was found to be less variable for thunderstorms than for slow-moving storms. Analysis of the areal distribution showed a large variability of total rainfall between stations, particularly for thunderstorms. Average rainfall for the basin was determined by weighting the average rainfall between successive isohyetals by the area between isohyetals, totalling these products and dividing by the total area. Figure 2 presents the isohyetals for the largest peak discharge (July 23, 1969).

Stream flow stage data are available from nine gages in the watershed operated by the USGS. However, records are sketchy for the purposes of this study due to the destruction of the gages during extreme flooding and delays in replacing the gages. Discharge rates for all of seven primary locations are available for only one of the seven flood events selected for the study.

Evaporation directly affects the available depression storage and therefore affects the proportion of rainfall which occurs as runoff. The evaporation rate used as input to STORM is the pan coefficient for the Washington area (0.76) published by the NWS extrapolated for winter months.

Definition of the Rainfall/Runoff Relationship

The hydrologic data described above for six storm events were used with data for present land use conditions to adjust the runoff coefficients used in STORM until the model reproduced field conditions within a preset margin. This procedure resulted in the definition of the rainfall/runoff relationship for the Four Mile Run Watershed and a calibrated simulation model that can be used to generate extended runoff records from the long term rainfall records at National Airport. The six storm events were selected for the calibration procedure on the basis of flood magnitude, recentness, and availability of rainfall and runoff data. All six storms had a recurrence interval greater than five years.

Land use data were transformed into percent surface imperviousness for each of five land use classifications: single family residential and schools, multi-family residential, commercial/office/institutional, industrial and open space. While the residential and open space classifications occupy 15.5 square miles of the total 19.5 square miles of the watershed, the percent impervious for residential usage ranges from 13 to 71 percent.

Determination of the runoff coefficient for pervious and impervious areas is the essence of the calibration process in STORM. The runoff coefficient is the fraction of the total rainfall which becomes surface runoff, and is thus directly related to the infiltration capacity of the surface. The runoff coefficients determined during the STORM calibration were, for pervious areas, 0.39 and, for impervious areas, 0.90. These values were then used in simulating the flood which would result from the design storm event. It should be noted that all six calibration storms caused major flooding; therefore the runoff coefficients are defined, in the strict sense, for flooding events only.

The model was calibrated using the complete hydrographs of two of the six major storm events and peak discharge measurements for the other four available for a downstream gage. Complete hydrographs for these four storms were not available due to the loss of the key downstream gage during the storms. As shown in Figure 3, the calibration simulations for discharges of five of the six storms showed agreement within ± 12 percent of measured flows. The discrepancy can be caused by several factors, most importantly that the model assumes that infiltration capacity of the surface is constant through the duration of a storm and that depression storage is constant for all storm magnitudes.

A sensitivity analysis was made for the model in order to determine the relative effects of varying key parameters, i.e., ratio of basin rainfall to National Airport rainfall, pervious and impervious runoff coefficients, depression storage, percent impervious for low density land use category and percent impervious for the vacant land use category. The sensitivity analysis showed that:

1. The predicted discharge rates are highly sensitive to inaccuracies in the average rainfall patterns for the basin,

2. Large changes in land use produce a significant change in peak discharge for major storm events,

3. The effects of land use changes over the calibration period (1963-1973) are overshadowed by inaccuracies in stream flow measurement, and

4. The sensitivity of the model to changes in land use is relatively independent of the runoff coefficients determined in the calibration process.

Analysis of Design Flood Frequencies

Flood frequency analysis was used to determine the probable extreme flow which the flood control project must accommodate. The specific flood frequency which serves as the basis of the project design must be selected through economic analyses and policy decisions. The expected flood frequency for flood events is determined by analyzing the statistical variation of historical flow records. Since the project design is based on present land use conditions, these historical flow records must be adjusted to account for the effects of urbanization. Figure 4 presents a comparative flood frequency curve developed by two methods--the unit hydrograph method with external flow adjustment (USACE method)[4] and rainfall runoff analysis for present land use (STORM method)

The USACE method for adjusting flow records was to increase historical flows by fixed annual percentages. The method used in the present study is based on discharges predicted by STORM, calibrated for present land use, and historical rainfall records. A comparison of the two methods shows a significant difference, but flow frequency curves for the methods cross near the 100-year recurrence interval which was the point selected as the design frequency. For intervals of less than 90 years STORM predicts higher annual flows and for intervals greater than 90 years it predicts lower peak annual flows. Since the predicted peak annual flows for these high recurrence intervals are projected from available records, the difference in the two methods for recurrence intervals greater than 60 years is a direct result of differences of predicted flows in the less frequent events. At a design recurrence interval of 100 years the peak annual flow based on the model STORM anlaysis is only 2.4 percent lower than the USACE design flow. That difference was judged to be insignificant for project design.

It should be noted that the STORM method was based on calibration to only flood events. Therefore, STORM overestimates minor annual floods.

Development of the Design Storm

A design storm event was developed in order to evaluate the effects of urbanization and runoff control on the USACE project. The channel design portion of the project was selected as the focal point of the study because it has a lower design capacity than any of the other flood control structures in the flood control project. Since the basis of the channel design is the 100-year flood, the design storm must generate such an event when it is applied to the existing watershed land use pattern.

The design storm event was developed by the method of Kiefer and Chu.[5] This method uses the rainfall intensity-duration curve to yield the fraction of the rainfall before the time of peak intensity which is equal to the ratio observed for the area. It gives a design storm consistent with the measured rainfall patterns and the results of several previous studies. The actual design storm used in STORM is a stepped hyetograph developed from the continuous function produced by the Kiefer and Chu method. Figure 5 presents the design storm that was adopted.

The design capacity of the channel proposed by the USACE is 22,500 cfs. The model STORM predicted a 100-year flow of 21,950 cfs using historical data. Using the Kiefer and Chu 100-year design storm, only 19,500 cfs was predicted. Therefore, the design storm rainfall was increased by a constant percentage to generate a peak runoff of 22,500 cfs. The frequency of the design storm thus produced therefore exceeds the 100-year rainfall return frequency by some small amount. Justification for this adjustment can be inferred from the distinction between rainfall frequency and flood frequency. The analyses in STORM, although they are based ostensibly on runoff, are really based on rainfall because of the limitations of the rational method. It is logical, therefore, to modify the design storm to reflect flow records instead of rainfall.

The Detailed Model, WREM

Unlike STORM, which does not include routing and considers the collection system only indirectly, the model WREM routes flow using the Navier-Stokes equation and requires a detailed description of the watershed, the sewer system and the stream network. A drainage area receives rainfall which is reduced by infiltration losses and by intercepted runoff (depression storage). Infiltration is estimated by equations relating the infiltration rate to the antecedent moisture conditions and to soil type. Standard SCS soil classifications are used and the infiltration rate modified according to rainfall intensity and timing. Infiltration occurs both on pervious and impervious areas, but at different rates.

Residential runoff from both pervious and impervious areas is further modified by retaining a small portion of the runoff on the surface. Retention depths ranging from 0.05 inch to 0.20 inch are used.

Runoff is then routed from each subcatchment using the Manning equation to portray overland flow. The average flow length of the pervious and impervious areas is estimated and the flow velocity estimated.

Runoff is collected at an inlet and conveyed by storm sewer or gutter downstream through the collection system. Manning's equation for open channel flow is solved by finite difference techniques to maintain continuity using average flows over a time interval usually ranging from 5 to 30 minutes.

Hydrographs are routed through the stream system by shortening the time step to 40 seconds and solving the transient flow equations at that time step by finite difference approximations. Tidal effects on the lower reaches are included.

The WREM Network

The watershed was subdivided into 177 drainage areas connected by 97 minor pipes. The main channel and minor tributaries are conveyed through an additional 90 channels and major pipes. The rainfall interval used is 15 minutes with records developed from 4 to 8 continuous gages depending on the storm event simulated. Nine major land use categories are used for the impervious/pervious estimation. The impervious/pervious data by land use category are developed for 49 zones within the watershed to incorporate geographic locational differences in lot coverage. Soils data revealed that 3 of the 4 SCS classifications occur in the watershed. These soil classifications are assigned to each of the 177 drainage areas. Intensive data collection was undertaken to define:

Rainfall variations (temporal and areal)

Soil type

Land use (past, current and future)

Soil cover (impervious/pervious data)

Storm sewers

Natural channels.

Calibration Storms

The watershed experienced major flooding events in 1963, 1966, twice in 1969, 1970, 1972 and 1975. The rainfall hyetographs were prepared for each of these storms from the rain gage network data. Streamflow data are unfortunately lacking as the 1969 storm destroyed the stream gage. Therefore, only peak flow measurements are available for the 1969 storms and all storms thereafter.

Surveying the available hydrologic data and comparing it to the available land use data resulted in the selection of 1963, (July) 1969 and 1972 floods as calibration storms. The land use breakdowns for each calibration year shown in Table 1 were prepared as were details of channel/storm sewer modifications. Antecedent moisture conditions were determined for each storm. The model was then used to simulate these three events. The model results are presented in Table 2 and compared to measured flow at defined points. The USGS gaging station at Shirlington is Transport Model Conduit #401 which drains 14.3 square miles of the watershed's total of 19.5 square miles. Agreement was good there for the two most recent storms (1969 and 1972). The other conduits are in tributary streams usually draining smaller tributary areas. The exceptions are 470 and 408 which are the box culverts under the RFP Railroad and the Mt. Vernon Avenue Bridge, i.e., downstream from the mouth. Peak flow estimates were available there.

Conclusion

This project has demonstrated the conjoint use of two models to utilize the best features of each. They have been used individually by many investigators throughout the country; this is the first time, so far as the authors are aware, that the models have been used together. WREM has provided the capability to examine the response of the system to a single design event in great detail. STORM has provided the hydrologic background to insure that the single event used is significant. Taken together, the models give the best of both continuous simulation and single event simulation.

References

1. "Urban Runoff: Storage, Treatment and Overflow Model 'STORM'," Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, California, September 1973.

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3. Baltimore District, Corps of Engineers, *Fourmile Run: Local Flood-Protection Project*, Design Memorandum No. 1, Hydrology and Hydraulic Analyses, June 1972.

4. Keifer, C.J., and H.H. Chu, "Synthetic Storm Pattern for Drainage Design," *J. Hydraulics Div., Proc. ASCE*, HY4, Vol. 83, August 1957, p. 1332.

TABLE 1

FOUR MILE RUN LAND USE

TYPE DESC.	1963	1969	1972	1975	FUTURE LAND
OPEN SPACE	4.0901	4.0395	3.9125	3.8318	3.5119
LOW DENSITY	8.3194	8.2601	8.2681	8.2652	8.3789
MEDIUM DENSITY	0.9754	0.9754	0.9754	0.9754	1.0242
HIGH DENTITY	2.3318	2.4133	2.4664	2.5474	2.0377
SCHOOLS	0.7207	0.7314	0.7996	0.7996	0.7996
INSTITUTIONAL	0.8319	0.8409	0.8466	0.8495	0.8068
COMMERCIAL	1.3058	1.3053	1.3050	1.3058	1.3156
INDUSTRIAL	0.5693	0.5693	0.5693	0.5693	0.5693
SHIRLEY HIGHWAY	0.2019	0.2019	0.2019	0.2019	0.2019

TABLE 2

FLOW CALIBRATION RESULTS AT USGS GAGING STATIONS

	1972			1969			1963		
Transport Model Conduit #	USGS Flow	Model Flow	Diff. %	USGS Flow	Model Flow	Diff. %	USGS Flow	Model Flow	Diff. %
218	--	1,107	--	1,530	1,981	↑29.6	--	1,290	--
217	980	795	↓18.9	1,280	1,287	↑ 0.5	830	944	↑13.7
219	--	5,550	--	4,800	6,317	↑31.6	--	5,915	--
310	700	651	↓ 7.0	1,600	1,279	↓20.3	--	772	--
308	1,250	843	↓32.5	1,900	1,775	↓ 6.5	--	779	--
401	10,000	9,372	↓ 6.2	24,600	24,213	↓ 2.6	11,700	9,292	↓20.6
506	--	8,853	--	--	13,183	--	--	8,822	--
416	--	1,637	--	2,200	3,040	↑38.2	--	2,186	--
415	--	784	--	1,700	1,308	↓23.1	--	1,018	--
408	--	10,861	--	17,000	17,265	↑ 1.5	--	11,780	--
472	--	6,124	--	5,500	6,250	↑13.6	--	5,752	--

-- Indicates Value Not Determined

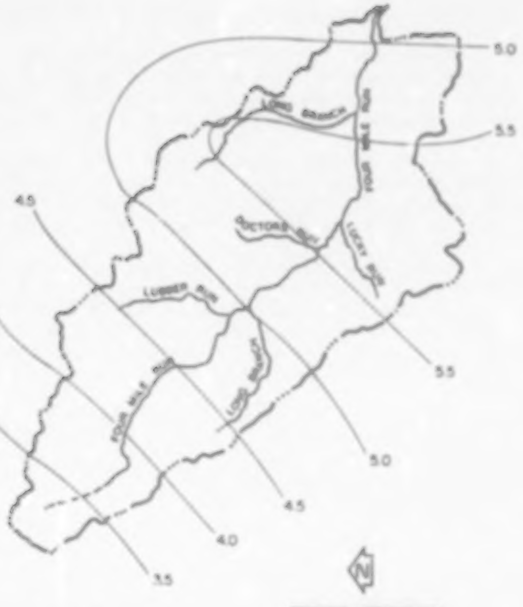
5.0
5.5
4.5
4.0
3.5
LONG BRANCH
FOUR MILE RUN
DOCTORS RUN
LUCKY RUN
LUBBER RUN
5.5
5.0
4.5
4.0
3.5
N
0
1
2 MILES
BASIN BOUNDARY

FIGURE 2

Areal Distribution of Total Rainfall for 700 EST July 22 to 1800 EST July 23, 1969

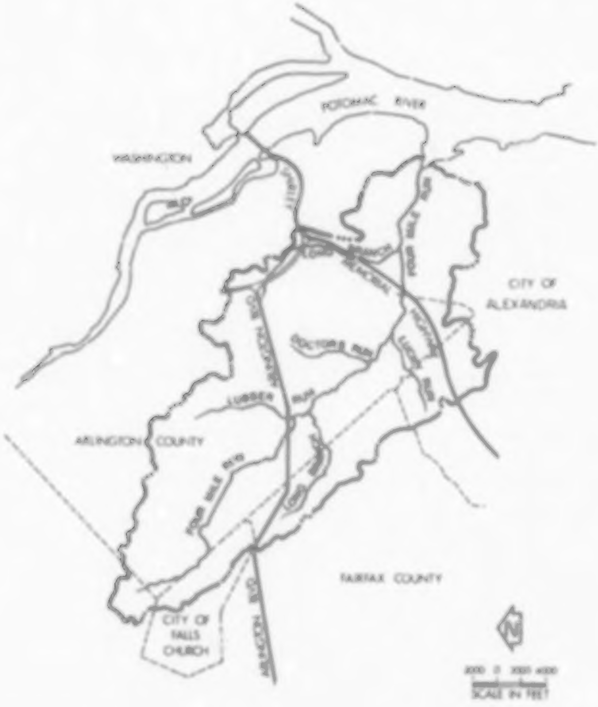
POTOMAC RIVER
WASHINGTON
CITY OF ALEXANDRIA
DOCTORS RUN
LUBBER RUN
ARLINGTON COUNTY
FOUR MILE RUN
FAIRFAX COUNTY
CITY OF FALLS CHURCH
ARLINGTON BLVD
N
2000 0 2000 4000
SCALE IN FEET

FIGURE 1

Four Mile Run Watershed Map

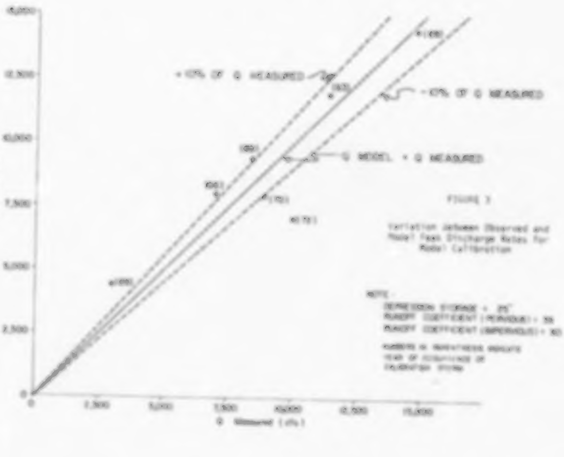

FIGURE 3

Variation between Observed and Model Peak Discharge Rates for Model Calibration

NOTE:
DEPRESSION STORAGE = .25"
RUNOFF COEFFICIENT (PERVIOUS) = .50
RUNOFF COEFFICIENT (IMPERVIOUS) = .90

NUMBERS IN PARENTHESES INDICATE
YEAR OF OCCURRENCE OF
CALIBRATION STORM

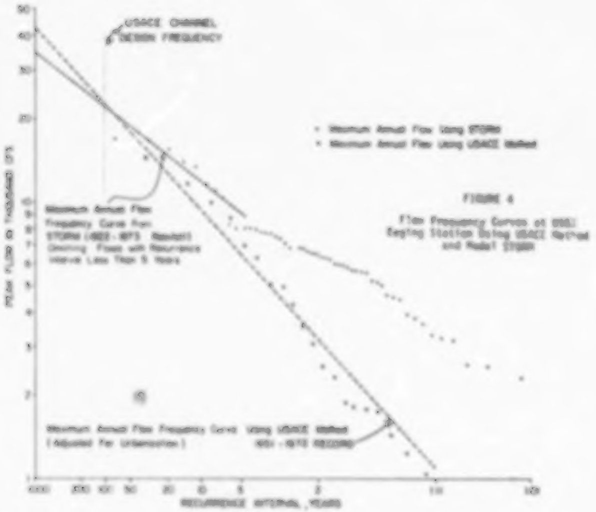

FIGURE 4

Flow Frequency Curves at USGS Gaging Station Using USACE Method and Model STORM

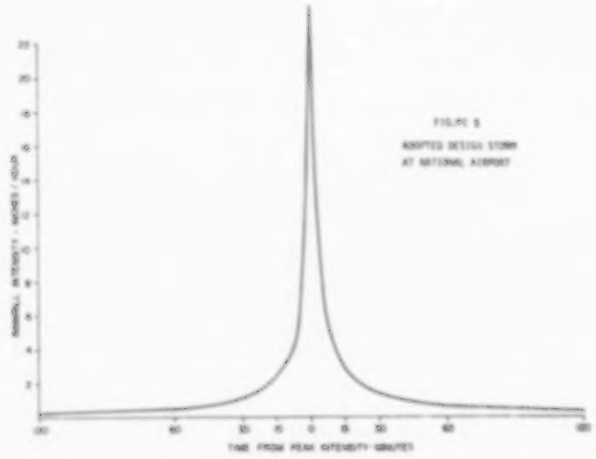

FIGURE 5

ADOPTED DESIGN STORM AT NATIONAL AIRPORT

PLANNING MODELS FOR NON-POINT RUNOFF ASSESSMENT

Howard A. True
Computer Systems Analyst
Ambient Monitoring Section
Surveillance and Analysis Division
E. P. A., Region IV, Athens, Georgia

ABSTRACT

Several computer based processes were developed for assessing the potential magnitudes of constituents from non-point sources. These processes have evolved from application of diverse procedures and literature data to solving specific problems in Environmental Impact Statement preparation and review, National Pollutant Discharge Elimination System* permit load allocations, and preparation of water quality field survey reports. The availability of workable processes used in industrial operations research and anticipated needs in the Section 208 areawide studies have led to the development of some very useful calculating procedures. The coverage of much of the vast spectrum of gross assessments amply justify the efforts expended to date. Major benefits can be derived by repetitive use of these processes to calculate relative numerical measures of effects resulting from changes in treatment level percentages, land use allocation percentages, population densities, loading rates, and rainfall event intensities.

These grouped processes are referred to as planning models and their formulation and data requirements are given in separate documentation. They are not excessively complex or costly to run and simple problems can be handled with a minimum of effort. Flexible inputs and external user controls allow maximum exercise of judgment by the user and presents the opportunity for imaginative and innovative problem formulation. Report exhibits and resource requirements are contained in the handout material.

BACKGROUND

An early review of P.L. 92-500, FWPCA** amendments, indicated that major emphasis would be placed on assessment of areawide pollutant sources. Historically, water quality planners have given primary attention to point sources and have developed few procedures for assessing impacts from diffused sources. Environmental Impact Statement (EIS) requirements have imposed a mandate on those responsible for preparation and review of Environmental Impact Statements to insure adequate coverage for all significant environmental impacts. EPA, Region IV, which covers eight southeastern states, has calculated the magnitude of non-point constituents for a number of federally prepared Environmental Impact Statements. These operational needs forced the development of assessment procedures for producing quick answers and have resulted in a fair degree of success. Analytical requirements have varied enough to require the development of several discrete calculating processes. In response to the requirements of the Section 208 areawide planning program, these procedures have been collected and formalized into a few processes capable of serving as planning models. No attempt has been made to duplicate existing stream, reservoir, estuary, and storm water management models.

GENERAL CHARACTERISTICS

The individual planning models discussed here are: (A) "Urban, Commercial, and Industrial Runoff," (B) "Erosion, Sedimentation, and Rural Runoff" and (C) "Total Loadings from Point and Non-Point Sources to Waterbodies." Models (A) and (B) produce independent reports and can also provide loading factors for model (C). Model (C) provides a composite report for multiple point and non-point sources for a single parameter. Urban areas can be split into twenty sub-areas and up to forty parameters can be calculated for single storm events within a metropolitan area using model (A). Large or small areas, such as entire river basins or single-acre plots, can be analyzed, using model (B), for soil loss, sediment delivered, and the usual rural parameters (Nitrogen, Phosphorous, Potassium, BOD, TOC, and Acid drainage). Best combinations of treatment requirements and land use alternatives can be determined by multiple runs with model (C). The hydrologic, transport, and calculating mechanisms differ in all processes, and each process is designed to best fulfill its intended purpose.

The "Urban, Commercial, and Industrial Runoff" Model (A)

This planning model is designed for a single rainfall event and will calculate the "first flush" slug load in pounds or coliform counts along with runoff concentrations for up to forty parameters at a time. These runoff slugs from up to twenty sub-areas are routed to a water body mixing zone, and the resulting stream or stillwater constituent concentrations are calculated after each slug arrives. Runoff water quantity is calculated in a manner similar to the "Rational Method" and all parameter calculations use deterministic methods.

Key parameter inputs to the model are: parameter name, units, waterbody background concentration, curb mile and per acre loading factors. Waterbody input information includes acre-feet for stillwater or ft^3/sec flow and velocity for moving streams. Other inputs include routing distances, runoff velocities, area, rainfall intensity, area type runoff factors, and either population for suburban areas or percent imperviousness for industrial and commercial areas. Multiple rainfall event intensities are allowed to give multiple reports for all areas in a single run.

Model features are:

(1) Utilization of the first fifteen minutes of rainfall only.

(2) Calculated curb miles and percent imperviousness, utilizing regression equations and population density, for suburban areas only.

(3) Summarization of curb mile loaded suburban areas with areal loaded commercial and industrial areas.

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* NPDES

** Federal Water Pollution Control Act

(4) Still water or moving stream mixing depending on receiving water input data.

Productive uses are:

(1) Gross assessment of current and projected area non-point pollution potential.

(2) Reasonably accurate calculation of urban type non-point loads after load factor adjustment consistent with sampling and local characterization of pollutants.

(3) Supplies refined, non-point loadings to Model (C) for consolidating point and non-point single parameter loads to waterbodies.

The "Erosion, Sedimentation, and Rural Runoff" Model (B)

This planning model is primarily of the periodic type and can be run for a single month or any group of consecutive months not exceeding one year. It is essentially nonhydrologic since the calculating mechanism is the "Universal Soil Loss Equation" developed by USDA. It will handle a single storm for erosion and sedimentation only, but special input requirements apply in this case. The model calculates tons of soil loss, sediment delivery to waterbodies and sediment downstream migration. Forest litter, nitrogen, phosphorous, potassium, BOD, TOC, and acid drainage are calculated and reported in pounds. Excluding acid drainage, the remaining common parameters are calculated from sediment, litter (leaves, twigs, etc.), and from animal and fowl droppings.

This is a probabilistic process using a random number generator to obtain a better representation of highly variable conditions. The process can easily be made into a pure deterministic process by using mean values and zero deviations in the input data. Some users have operated in this manner successfully. The internal design of this process is quite complex and changes other than report line formats are likely to lead to disaster and are not recommended.

No provisions exist for handling pesticides; however, model (A) will calculate these parameters when operated with areal loading factors for pesticides. Model (B) is designed to give the user almost total control of results through localized input data and its flexibility allows a minimum of input with a default to national distributions and loading factors contained internally or in the master deck preceding local data.

Key inputs to this system include: report headings, time period, multiplier starting value for the random number generator, standard state FIPS numbers, and number of units. Each sub-area requires: acres, blowup factor (plot size), one to five soil types, percent slope and slope length range, one to five crop management practices, one to five erosion control practices, load factors for sediment and litter, animal and fowl counts, and loading factors for acid drainage.

Model features are:

(1) Multiple sub-areas within each state for detailed definition.

(2) Multiple number of states for handling entire river basins.

(3) Gross assessments for large areas with minimum local input data needed.

(4) Very detailed assessments for areas of interest by using many small units and comprehensive localized data.

Productive uses include:

(1) Projections of effects of land use changes and erosion control practices with minor changes to input data.

(2) Refining load factors for model (C) for use in consolidating point and non-point single parameter loads to waterbodies.

The "Total Loadings from Point and Non-Point Sources to Waterbodies" Model (C)

This planning model uses some concepts from R. A. Vollenweider's "Export Process" and has no hydrologic characteristics. The time period can be from one day to any number of days, such as a one-hundred-and-fifty day growing season. All loading factors are on an annual basis and are modified by the factor (period in days/365). The model is designed to handle a single parameter for three point sources and five non-point sources for each of an unlimited number of sub-areas. The composite report gives three columns of loading information composed of minimum expected, most probable, and maximum expected. The minimum and maximum quantities are calculated from loading factor limits. Probabilistic methods, utilizing a random number generator, are used to calculate the most probable quantity from each source.

This model is a relatively simple process and the computer program can be modified by users if desired. Any parameter that is quantifiable on a weight basis can be handled. Simple attenuation processes are built into the system.

Key inputs to this system include: report headings, time period, modification to multiplier starting value for the random number generator, population, acres, treatment level percentages for point sources, land use distribution percentages for non-point sources, loading factor limits (national and localized) and attenuation factors.

Model features are:

(1) Unlimited number of sub-areas.

(2) A set of national loading factor limits for default use in the absence of local loading factor limits.

(3) Capabilities for producing a composite report from multiple point and non-point sources for a single parameter.

Productive uses include:

(1) Determining load allocations for issuing NPDES permits by making multiple runs using modified point source treatment levels and setting each sewage treatment plant up in a separate sub-area.

(2) Making long range projections by changing population, treatment level percentages and land use distribution percentages for certain sub-areas.

(3) Gross assessments to determine if a more detailed study is needed requiring use of models (A) and (B).

(4) Producing progress reports.

SUMMARY

The main objective in assessing non-point runoff is to estimate constituent loads for some representative time period for a defined drainage area. No absolutely accurate answers appear economically feasible now or in the near future, and getting a handle on the many facets of the problem is very difficult. These planning models are generalized tools designed for initial gross assessments with refinement capabilities to provide ball park numbers for decision making. Numerical values such as these, systematically arrived at, provide a basis for estimating the relative effects of changes to physical features. Control of runoff constituents through process and/or structural changes would settle, filter, or otherwise reduce concentrations rather than eliminate runoff. This is often in direct conflict with some forms of flood control where speeding up the runoff from land is the paramount objective.

The accuracy of output from these planning models is directly related to the quality of input data supplied by the user. These models are tools for planners and are being made available to anyone willing to learn how to use them.

All computer programming is in the universally used FORTRAN-4 language. Source programs and test case run decks for all three planning models are in library files on the EPA-OSI computer system and may be reproduced on 80-column cards if a request is made through normal EPA channels. Run modules for each planning model can be accessed by EPA-OSI users through Job Control Language procedures. Concise documentation for problem definition and data coding is contained in the exhibit handout.

All libraries are located on EPA-OSI disk RIV004. Source programs and exhibit run decks (approximately 1,450 cards) are in a library named CNMD01.HAT.NPPROG and the exhibit run decks only (256 cards) are in a library named CNMD01.HAT.NPRUN. Compiled modules are in a library named CNMD01.HAT.ASSESS and program names are EPAURA, EPARRB, and EPATLC for planning models A, B, and C.

DESIGN AND APPLICATION OF THE TEXAS EPISODIC MODEL

John H. Christiansen
Data Processing Section
Texas Air Control Board
Austin, Texas

Summary

The Texas Episodic Model (TEM) is a new short-term air pollution dispersion computer model being used extensively by the Texas Air Control Board.

Design innovations make the TEM several times faster than models of comparable sophistication and accuracy. The TEM uses steady-state bivariate Gaussian plume point source logic, but solves the dispersion equation by interpolating in a table of precalculated coefficients, rather than time-consuming explicit calculations of the exponentials involved. Area sources are handled by a very fast algorithm based on work of S.R. Hanna and F.A. Gifford.

The model calculates plume rise via one of six equations (all due to G.A. Briggs), choosing the appropriate equation on the basis of 1) downwind distance, 2) atmospheric stability, and 3) whether the rise of the plume is dominated by thermal buoyancy or momentum. It also takes into account pollutant decay, variation of wind speed with height, and atmospheric inversion layers. Plumes may be trapped below an inversion or may penetrate it and escape. The degree of penetrability is variable, and is specified by the user, allowing simulation of "weak" or "strong" inversions.

Concentrations are calculated for one or two pollutants at up to 2500 locations in a uniform grid of arbitrary dimensions and spacing, for a wide range of sample times from 10 minutes to 24 hours.

The versatility provided by a wide variety of input options and graphic output options allows the TEM to serve the needs of several different user groups within the Texas Air Control Board. Four examples of current TEM applications are discussed.

Introduction

The Texas Episodic Model, or TEM, is a FORTRAN computer program which may be used to predict air pollution concentrations for short time periods. An emissions inventory and a set of meteorological conditions are used to create scenarios simulating the dispersion of airborne pollutants in the lower atmosphere. The TEM was developed to fulfill the requirements of the Texas Air Control Board (TACB) for a model of high enough efficiency, sophistication, and versatility to make it a worthwhile analytical tool for a wide range of applications.

This paper will first describe several design features of the TEM. The input data required and the types of output available will also be discussed. The remainder of the paper will deal with some of the TEM's current areas of application within the TACB.

Model Design

Point Source Algorithm

The TEM employs the steady-state Gaussian plume hypothesis for calculation of concentrations due to point sources. This hypothesis makes use of the following assumptions:

1. The emission rate of the source is constant, and no dispersion occurs in the downwind direction. The pollutant is simply transported downwind at the appropriate wind speed. The TEM uses the wind speed at the physical source height.
2. In both the crosswind and vertical directions, the pollutant is dispersed by turbulent eddy diffusion. The concentration patterns in these directions take the form of Gaussian distributions about the center line of the plume. The standard deviations of the two Gaussian distributions increase with downwind distance or time elapsed since release. In the TEM, the standard deviations are power law functions of downwind distance.
3. The plume is reflected at the earth's surface. This means that none of the pollutant is lost to reaction or deposition at the surface.

Pollutants are assumed to be essentially non-reactive. For concentrations at ground level, the Gaussian plume equation may be written:

$$\chi = \frac{10^6 Q}{\pi U \sigma_y \sigma_z} \exp\left[\frac{-H^2}{2\sigma_z^{\,2}}\right] \exp\left[\frac{-y^2}{2\sigma_y^{\,2}}\right] \qquad (1)$$

where χ is the concentration, in micrograms per cubic meter;
Q is the source emission rate, in grams per second;
U is the wind speed at physical source height, in meters per second;
H is the effective source height, equal to the physical source height plus the plume rise, in meters;
x,y,z are the downwind, crosswind, and vertical directions respectively, in meters.

The standard deviations σ_y and σ_z vary with downwind distance x and atmospheric stability class S according to the following formulae:

$$\sigma_z = a(S)\, x^{\,b(S)} \qquad (2)$$

$$\sigma_y = c(S)\, x^{\,d(S)} \qquad (3)$$

Values of the stability-dependent coefficients a,b,c, and d are derived from Turner[1] and Busse and Zimmerman[2].

Vertical Wind Profile. The mean wind speed in the lower atmosphere typically increases with height in a way that can be approximated by a power law. The quantity U in equation (1) represents the wind speed at the physical height of the source. The TEM derives this wind speed for each source from the input "ground level" wind speed by a formula featuring exponential increase with height, with the exponent dependent on atmospheric stability.

Plume Rise. The effective source height, H, in equation (1) is the sum of the physical source height, h, and the plume rise, Δh. Calculation of the plume rise is handled quite rigorously by the TEM. The plume may emerge into "stable" (stability classes E and F) or "unstable" (classes A through D) air. The dimensions, exit velocity, and exit temperature of the source and the ambient temperature will indicate whether the upward motion of the plume is dominated by momentum or thermal buoyancy. The TEM employs a separate set of plume rise equations for each of the four possible situations: stable/buoyant, stable/momentum, unstable/buoyant, and unstable/momentum. The atmospheric stability is an input parameter for each TEM weather scenario, so for each source the program has only to decide whether the plume rise is momentum- or buoyancy-dominated. Peak plume rise is calculated using both the momentum and buoyancy plume rise equations for the atmospheric stability in question. If the momentum equation yields a higher plume rise than the buoyancy equation, the plume is assumed to be momentum-dominated, and the momentum plume rise is used. If the buoyancy plume rise is higher, it is used instead.

An additional equation is used to calculate plume rise as a function of the downwind distance out to the distance at which the plume reaches maximum height. The six plume rise equations used by the TEM are all due to Briggs[3].

TEM Solution of the Dispersion Equation. The TEM is able to solve equation (1) very quickly for each source-receptor combination due to a numerical trick first introduced in the Texas Climatological Model[4]. Let K_y and K_z be defined by

$$K_y = \frac{1000}{\sigma_y} \exp\left[\frac{-y^2}{2\sigma_y^2}\right] \qquad (4)$$

and

$$K_z = \frac{1000}{\pi\sigma_z} \exp\left[\frac{-H^2}{2\sigma_z^2}\right] \qquad (5)$$

Then, from equation (1),

$$\chi = \frac{QK_yK_z}{U} \qquad (6)$$

Note that K_y and K_z are independent of emission rate Q and wind speed U.

In a separate program, K_y values were generated for twenty downwind distances, x, eight angular distances from the plume centerline, θ ($y = x\tan\theta$), and seven stability classes, S. The K_y values for each of these 1120 combinations (20x8x7) are stored as data tables in the TEM. Similarly, K_z values were generated for the same twenty downwind distances, fourteen effective source heights, H, and seven stability classes, giving 1960 values The downwind distance values chosen were x=2,3,4,5,6 7,8,10,12,14,17,20,23,27,31,36,41,47,53 and 60 km. The effective source heights were H= 10,20,30, 50,70,100,150,200,300,450,700,1000,1400 and 2000 meters. The seven stability categories are commonly referred to, in increasing order of stability, as classes A,B,C,D (day), D(night), E, and F. Finally, the angular distance from the centerline were $\theta = 0, \delta, 2\delta, \ldots, 7\delta$, where the increment δ is a function of stability class, ranging from 5° for A stability to just 1° for F stability. This means that the K_y data table is good to an angle of 35° from the plume centerline in A stability, but only 7° in F stability. The δ values were chosen so that the concentration at an angle of 7δ from the centerline would be 1.0 percent or less of the centerline concentration at all downwind distances. As stability decreases, the effectiveness of turbulent diffusion increases, so that the plume spreads out more and a larger δ is required.

For downwind distances greater than 2.0 kilometers, the TEM calculates point source concentrations from equation (6) instead of equation (1). K_y and K_z are found by linear interpolation in the K_y and K_z tables. This procedure is much faster than the explicit calculation of the exponentials in equation (1), and is chiefly responsible for the high speed of the model. For downwind distances of less than 2.0 kilometers, the TEM uses equation (1) instead of equation (6). This is because the accuracy of the linear interpolation is inadequate at such short distances.

When interpolating for a K_z value, it is assumed that the plume has completed its rise, so that the effective source height is constant in the distance range under consideration. The rise of the plume is considered to be complete before the plume gets 2.0 kilometers downwind of its source, a valid assumption in nearly every case.

Mixing Height. The "mixing layer" of relatively turbulent air near the ground is very frequently bounded by a layer of stable air aloft. The distance from the ground to the bottom of the stable layer is the "mixing height". The effect of the stable layer is virtually to prevent vertical dispersion above the mixing height. Pollutants emitted into the mixing layer will be trapped there, eventually becoming totally mixed in the vertical direction. On the other hand, pollutants emitted directly into the stable layer will remain there, and not disperse downward to any extent. The TEM can simulate either of these possibilities. If the physical source height exceeds the mixing height, the plume will obviously emerge into the stable layer, and the source is neglected. If the maximum effective source height is less than the mixing height, the plume is trapped in the mixing layer, and the expression for vertical dispersion (K_z) will have to be modified to account for it.

The TEM treats restricted vertical mixing as suggested by Turner[1]. Uniform vertical mixing impends at some downwind distance x_m (a function of σ_z), and is considered complete at $2x_m$. For $x \geq 2x_m$, equation (1) may be written

$$\chi = \frac{Q}{\sqrt{2\pi}\sigma_y LU} \exp\left[\frac{-y^2}{2\sigma_y^2}\right] \qquad (7)$$

with mixing height =L, and the Gaussian distribution in z replaced by a uniform distribution in z, $0 < z < L$. The corresponding form of equation (5) is simply $K_z = 398L$. The TEM uses equation (1) for $x \leq x_m$, equation (7) for $x \geq 2x_m$, and an interpolation between (1) and (7) for $x_m < x < 2x_m$.

A third possible situation is that of a source whose physical height is below the mixing height, but whose calculated effective source height exceeds the mixing height. Whether the plume escapes the mixing layer depends on how much larger the effective source height is than the mixing height, and on the strength of the inversion. The TEM simulates the effect of inversions of various strengths by introducing an inversion penetrability factor, I. A plume escapes the mixing layer if the calculated maximum effective source height is greater than the product of the mixing height and the inversion penetrability factor, $H > LI$.
For the weakest possible inversion, I=1. For a strong inversion, $I > 2$. A recent paper by Briggs[5] addresses the inversion penetration problem in considerable detail. If $LI \geq H > L$, then H is set equal to L, and the plume does not escape.

Pollutant Decay. Removal of pollutants from a plume by various processes such as adsorption and chemical reaction may be simulated (albeit simplistically) by assigning a decay half-life to each pollutant. The TEM adds a decay term to the dispersion equation (6):

$$\chi = \frac{QK_yK_z}{U} \exp\left[\frac{-0.692x}{UT_{1/2}}\right] \qquad (8)$$

where $T_{1/2}$ is the half-life, in seconds. Since half-lives of many pollutants may be dependent on meteorological conditions, separate half-life values are input to the model for each pollutant in each weather scenario.

Area Source Algorithm

The TEM's area source logic is based on an algorithm of Gifford and Hanna[6]. It uses the standard formalism of a grid of square area sources of the same size, but varying emission rates. The concentration due to area sources in a given square is due to the emissions in that square and in the N squares upwind.

The concentration is given by

$$\chi = \sqrt{\frac{2}{\pi}}\,\frac{(\Delta x/2)^{1-b(S)}}{U_o a(S)(1-b(S))}\left\{Q_o + \sum_{i=1}^{N} Q_i \left[(2i+1)^{1-b(S)} - (2i-1)^{1-b(S)}\right]\right\} \quad (9)$$

where Δx is the area source grid spacing in meters,
Q_o is the area emission rate of the square containing the receptor, in gm/km^2/sec,
Q_i are the area emission rates of the N upwind sources,
U_o is the surface wind speed, in meters/sec,
and a(S) and b(S) are as defined in equation (2).
The stability class index S is decreased by one (index for stability class A=1, B=2,...,F=7) to simulate urban surface roughness. In the TEM, the value of N is four, so each area source square affects itself and the four squares downwind of it.

TEM Inputs and Outputs

Input Structure

Input to the TEM can be divided into four sections, as listed below:

1. Control Parameters (4 cards). Control parameters remain constant throughout the run regardless of changes in weather in different scenarios. They specify such items as input and output options and dimensions and spacing of the grid of receptors at which concentrations are calculated.
2. Scenario Parameters (1 to 8 cards). From one to eight weather scenarios may be created in each run. Each scenario uses the same sources and receptors, but different weather conditions. Each card contains the necessary weather parameters for one scenario.
3. Area Sources (0 to 200 cards). Each area source card contains the location, dimensions and emission rates of one area source.
4. Point Sources (0 to 300 cards). Each point source card contains the location, height, diameter, exit temperature, exit velocity, emission rates and identification for one point source.

The control parameters give the user considerable flexibility in deciding what the model should calculate and in what form the results should be presented. A few of the more important ones will be mentioned here.

The TEM will calculate pollutant concentrations for one or two pollutants at up to 2500 locations ("receptors") in a rectangular grid of arbitrary dimensions and arbitrary but uniform spacing between rows and columns. The "receptor grid" is completely specified by five parameters: the coordinates of the southwest corner of the grid, the number of rows and columns (maximum of 50 each), and the spacing between rows and columns. An option allows the user to let the TEM calculate the grid parameters itself, choosing them so as to ensure that the point of maximum concentration for the entire source distribution, as well as the individual maximum for each source, will fall within the boundaries of a receptor grid of maximum allowable resolution.

The values of σ_y and σ_z in the dispersion equation were derived for a sample time of 10 minutes. The concentrations calculated by the TEM are thus 10-minute values, but they may be converted to 30-minute, 1-hour or 3-hour readings by a statistical formula dependent on atmospheric stability[7,8]. In addition, a 24-hour time period can be simulated using eight scenarios representing 3 hours of weather each.

The user has a choice of formats and units for source and weather data.

The concentrations of each pollutant at each point in the receptor grid can be displayed in any of the following forms, or in virtually any combination of them:

1. List of the coordinates and concentrations at each receptor. This is the standard form for most air quality models.
2. Map of the receptor grid. The concentrations across the receptor grid are displayed in two dimensions with coordinates along the edges of the page. Spatial concentration distributions are immediately apparent with this option.
3. Control list. As an aid in formulating control strategies, a list is printed of the identifications and contributions of the five point sources contributing the most to the total concentration at each receptor, for a maximum of 625 receptors (a 25x25 grid).
4. Finally, the coordinates and concentrations at each receptor can be output on punched cards for input to a contour plotting routine.

Notes on TEM Performance

To assess the relative speed of the TEM, several timing tests were conducted against the other two short-term models available to the TACB, with each model operating on identical sources and receptors. The two models, both of which are substantially less sophisticated than the TEM, are the Argonne Steady-State Model (ASSM), and the Small Area Model MK IV, developed some years ago by the TACB. The TEM proved three to five times faster than both models. The larger the area covered by the simulation, the faster the TEM will be, since it uses a faster algorithm for downwind distances over 2.0 kilometers. The error introduced by K_y and K_z interpolation is typically on the order of 1.0 to 5.0 percent.

TEM Applications

The TEM has found several areas of application within the Texas Air Control Board. Although the bulk of all TEM run requests come from the Meteorology and Permits Sections, each modeling study cited here originated in a different section of the TACB.

In the discussion of each application, the emphasis will be on the subject of the analysis, the TEM's role in the analysis, and the impact of the model results.

Permits Section

The TACB's Permits Section employs the TEM routinely as part of its analysis of new construction permit applications from Texas industries. Action taken on a permit application involving any potentially significant air pollution sources is governed by four basic criteria:

1. State and Federal allowable in-stack pollutant concentrations.
2. State allowable ground-level concentrations based on emissions from a single company or companies with contiguous properties.
3. Federal allowable ground-level concentrations based on all emissions in the area and background concentrations, if any.
4. Ground-level concentration of one percent of the threshold limiting value (TLV) for any compound having a TLV. These include about 500 compounds considered to have harmful health effects.

The TEM is used to evaluate the impact of the proposed new facility against the second and third criteria, and may in the future be used for the fourth as well.

The pollutants usually modeled are sulfur oxides (SO_x), and less frequently, total suspended particulate matter (TSP). Area sources are not used, and point source and receptor grid parameters are input in English units. The number of sources and the dimensions of the receptor grid vary greatly. For studies of a single plant (criterion two), there are generally from one to thirty sources, and a spacing between adjacent receptors in the receptor grid of 100 to 500 feet. For studies of the impact of the plant on the air quality of an entire region (criterion three), there may be from 30 to 300 sources, with a grid spacing of 500 to 2000 feet. An example of the latter is the basic inventory of 268 sources for the Houston Ship Channel, Texas' most heavily industrialized area. A typical receptor grid for this region would consist of 50 rows and 25 columns spaced 2000 feet apart, giving an area of roughly 10 by 20 miles, uniformly covered by 1250 receptors.

For each permit study, the Meteorology Section provides an ensemble of weather scenarios representing reasonable worst-case conditions for the area in question. From 4 to 100 scenarios (run up to eight at a time by the TEM) are usually necessary to complete a study. The number of scenarios run is largely dependent on the complexity of the source distribution. Also, if the TEM predicts a violation of an air quality standard, more runs will be made in order to assess the magnitude of the problem, and still more runs may be made using source inventories altered to reflect alternate approaches and control strategies for preventing the violation. If a significant violation of state or Federal standards is predicted, the permit application will be denied unless the necessary abatement procedures are instituted. If a minor violation is predicted, the applicant will be required to take precautions against its occurrence. The granting or denial of a permit on the basis of criteria two or three is thus very strongly dependent on the results of TEM predictions.

Air Quality Evaluation Division

The TEM is also being applied in a study undertaken by the TACB's Air Quality Evaluation Division (AQE). The study is attempting to establish culpability for violations of the 24-hour ambient air quality standard for total particulate by making use of the TEM's control list output option. The methodology is as follows:

1. A computer program searches the AQE master file of measured pollutant concentrations for receptors reporting a violation of the 24-hour standard. In general, when a region shows a violation, roughly five to eight receptors exceed the standard. The program then retrieves the weather data for the same day at a reliable weather station in the region. The weather data is in the form of eight 3-hour readings.
2. A 24-hour simulation is run with the TEM, using eight 3-hour scenarios drawn from the weather data and the best available inventory of point and area sources of TSP for the region in which the violation occurred. The control list option is used, giving the five sources contributing the most to the total concentration at each of up to 625 locations. Grid spacing is typically 0.5 to 2.0 kilometers. The source inventories for the Dallas and Houston areas contain roughly 100 area and 250 point sources each.
3. The predicted and observed concentrations are compared. If the predictions are within ± 30 percent of the measurements, the control list is consulted to see if any sources stand out as major polluters. If any such sources are found, consideration will be given to rewriting the local emissions regulations to prevent future violations. If the TEM grossly underpredicts the concentration, a search is made for poorly sited receptors (wind flow obstructions, etc.) and for unreported sources. Most of these searches have been successful.

This study is thus providing a check on the validity of receptor data and the completeness of the emissions inventory as well as determining culpability for violations of air quality standards.

Meteorology and Planning Sections

Texas' control strategy work for EPA's 10-year Air Quality Maintenance Plan (AQMP) is being undertaken by the Meteorology and Planning Sections of the TACB. The necessary dispersion modeling of sulfur oxides and particulates in designated Air Quality Maintenance Areas is performed by the TEM and the Texas Climatological Model (TCM), a long-term companion to the TEM with compatible inputs and outputs. The basic goal of the AQMP is to assure acceptable air quality through 1985, despite industrial growth, population growth, and changes expected in land use and availability of different fuels. The emissions inventories for each Air Quality Maintenance Area are extrapolated for future years, and the TEM is run with the control list option and an ensemble of possible short-term, worst-case weather scenarios to predict future air quality, to identify potential trouble spots and to aid in formulating control strategies.

Laboratory Division

The TACB's Laboratory Division is currently involved in a project which uses an extensive field study and TEM modeling to investigate the relationships between gaseous and particulate pollutants. In June and September of 1975, over sixty high-volume particulate samplers in the Houston area took readings simultaneously on nine different days. X-ray fluorescence analysis of the particulate matter collected yielded concentrations of chlorine, ammonium, nitrates, sulfates, total sulfur, benzine-soluble hydrocarbons, and several metals.

A substantial amount of sulfur in the form of sulfates and sulfites appears in the particulate samples. It is suspected that much of the sulfur was actually emitted in the form of sulfur dioxide. Since SO_2 is acidic, the sulfur could be tied up in the form of sulfites on contact with any alkaline particulate. TEM modeling is being used to help test this hypothesis The TEM is making 24-hour predictions of SO_2 and TSP concentrations across the Houston area for each of the nine days of the field study. If the hypothesis is valid, one would expect to find receptors where predicted TSP is less than measured TSP, predicted SO_2 is high, and the TSP collected contains large amounts of sulfur. The extent of conversion of SO_2 to particulates is probably dependent on travel time from source to receptor. Travel times can be approximated, since the wind speed is supposedly known and the TEM control list can identify the major contributing sources at each receptor.

Results of this project could have great impact in at least two areas. First, control of sulfur oxide emissions might be necessary to meet particulate standards. This should be reflected in the local regulations. Second, if the phenomenon mentioned above exists, it should be taken into account in dispersion models, at least in terms of adjusted decay rates and/or "calibration factors" if no better method can be found.

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AIR MODELING IN OHIO EPA

John C. Burr
Environmental Assessment Section Chief
Ohio EPA
Columbus, Ohio

A. Ben Clymer
Consulting Engineer
Columbus, Ohio

Annual Mean SO_2 and TSP Over Flat Terrain

Modeling for Ambient Network Design

The term ambient network is intended to mean that network which is used for assessing long-term concentrations as, e.g., annual mean concentrations for comparison with annual air quality standards. Urban background carbon monoxide concentrations are another example.

In this case one wants to know the mean concentration distribution of a pollutant over some area of concern. In other words we want to determine a three-dimensional concentration surface. The design problem then becomes one of determining the number and location (geographic) of sensors adequate to define such a surface with a specified degree of confidence. The design theory of such a network has been developed by the authors.[1,2] It utilizes a parametric representation of concentration as a function of distance. For pollutants originating from point sources a polar coordinate system is used, and the concentration representation is a gaussian function of the coordinate.[1-3] The theory has been applied to three cities in Ohio. The number and distribution of sensors, so determined, is reasonable.

Existing Models for Design of Regulations

Annual models currently being used by us are the Modified Climatological Dispersion Model (MCDM),[4] and the Ohio County Annual Maximum (OCAM) model.[5] Both MCDM and OCAM are steady-state, uniform wind, gaussian dispersion models. MCDM is a revision of CDM[6] which has been modified to generate a source contribution table.

We use MCDM because it has been shown, when properly applied, to produce reasonable correlation coefficients (range of 0.75 to 0.85). It is being modified to produce "coupling coefficients" which are merely row vectors of relative source contribution at each receptor. Thus a simple matrix multiplication of emission rate and "coupling coefficient" will predict the concentration at the receptor. In this manner we can easily examine the effect of altering various emission rates.

The OCAM model was developed to permit efficient and realistic modeling of maximum annual concentrations in smaller metropolitan areas. It treats both area and point sources. Area sources are modeled by the method of Miller and Holzworth.[7] It has been found[8] for point sources, that maximum annual concentration, normalized for emission rate, is related to mean plume height by a power law. The law is deduced from hypothetical source CDM modeling. OCAM includes a quantitative means of how a given source is to be modeled, i.e., as a point source or as part of the area sources.

Early application of OCAM for modeling sulfur dioxide yielded a correlation coefficient of 0.78 when based upon modeling in 36 Ohio Counties.[5] When extended by a Larson Transform[9] the OCAM model predicted second-highest 24-hour concentrations in these same 36 counties with a correlation coefficient of 0.66.

Matrix Model of Concentration by Source Category

This is a model with which we are experimenting. The emission rates are categorized according to a column vector, E,(m x 1) by Source Industrial Classification (SIC) codes. A matrix of constants, D,(n x m) relates SIC classified emission rates to an observed concentration column vector, C(n x 1):

$$\begin{matrix}\uparrow\\ n\\ \downarrow\end{matrix}\left\{\; C \;\right\} = \left[\begin{matrix} D \\ n \times m\end{matrix}\right]\left\{\; E \;\right\}\begin{matrix}\uparrow\\ m\\ \downarrow\end{matrix}$$

The n x m matrix D can, in principle, be determined from a least squares fit of historical data. Alternatively it could be synthesized from the "coupling coefficients" between sources (by SIC code) and receptors.

If the emissions are projected by SIC code, then the above matrix equation gives a forecast for the concentrations. It is also possible to invert the equation, in order to solve for a unique set of emissions, {E} which will yield a given set of concentrations {C}.

This is a highly condensed city pollution model. Its simplicity and potential ability for short-circuiting disperson modeling commend it for consideration.

Annual Mean SO_2 and TSP Over Nonflat Terrain

Phenomena of Concern

Nonflat terrain gives rise to a remarkable number of micro-and mesoscale meteorological phenomena affecting the dispersion of pollutants.[10-12] It would be valuable to be able to deal with the majority of these effects upon concentration at an arbitrary surface point. Among these effects are the following:

1. Channeling of wind by a valley, causing a strongly bimodal wind rose;
2. Boundary layer instability effects, such as vortex (eddy) and downwash generation on the lee side of a ridge;
3. Plume impingement on a ridge or plateau;
4. Increase of turbulence aloft due to surface roughness over a wide range of scales;
5. Downflow of colder air in a valley;

6. Irregular distribution of updrafts due to insolation of rough terrain;
7. Several possible effects of the thermal structure $T(z)$ of the atmosphere, including an elevated or ground-level inversion;
8. Extra turbulence due to wind shear;
9. Bending of plume by variation of wind direction with altitude;
10. Nonuniform wind speed and direction due to potential flow over rough terrain;
11. Possibility of a Coriolis effect in a large valley;
12. Reduction of wind speed in a valley relative to geostrophic wind;
13. Elevation of a "cloud" of pollution which is caused by inflow of cooler cleaner air below.

Analytical Approaches

The simplest assumption is to ignore terrain unevenness, as in all flat-earth models. The resulting errors are not well understood in cause or magnitude. If the terrain is very rough, the annual average concentrations predicted by a flat-earth model cannot be "calibrated" satisfactorily to observed data at a set of monitoring sites, because the scatter is so bad.

The next simplest assumption useful in the case of a ground level receptor which is elevated relative to the base of a source stack, is that the effect of nonflat terrain may be taken into account by deducting from stack height the elevation of the receptor above the stack base. In effect, this assumption is that the elevated ground is permeable to the wind and that the wind field is not distorted by the terrain. A somewhat more rational correction to plume height above rough terrain is made in the PSDM program.[12]

Since roughness of terrain greatly increases the diffusion coefficients σ_y and σ_z, an appealing model assumption would be that there is perfect mixing within some specified box, with flowthrough being determined by the wind. The authors have found that such a model, even with substantial dilution by exchange of air at the top, gives much too high a concentration at the ground, when applied to the valley area of Steubenville, Ohio.

Part of the modeling problem is to describe the wind vector field for each of a set of wind speed and direction classes. There are many approaches for finding the wind field, such as the shallow fluid model[13], closed-form approximations in simple geometries[14], and various numerical methods based on the Navier-Stokes equations[14,15] or modified potential flow.[16]

After having the wind field, one can apply one of the existing models, such as CDM[6], as a subroutine in a program which deals with pollution transport, diffusion, and decay in a nonuniform wind.[17] The authors are currently investigating this approach.

Diurnal Scale Problems

Modeling for Episode Network Design

An episode network has the purpose of detecting an incipient episode of high pollutant concentration over a period of days. The detection is only possible with some particular degree of confidence when performed by a given number of sensors, because the "signal" is "noisy". The statistical theory involved has been worked out by Clarenburg.[18] One of us (JCB) has extended the theory,[2] and we have applied it to two cities in Ohio.[3,19] The numbers of monitors thus determined are reasonable.

Diurnal Phenomena

The most disastrous air pollution episodes are those which last only a few days and which importantly involve short-term phenomena. These phenomena must be modeled, in order to understand how an area's pollution compares with short-term standards under various conditions. The modeling problems associated with these diurnal phenomena may be summarized as follows:

1. Inversions. The creation, persistence, and the diurnal rise and fall of an inversion are basic in pollution episodes, since they limit the mixing volume. Moreover, the production and maintenance of an inversion are correlated with low wind speed, which further increases pollutant concentrations. The modeling problem is to represent the vertical transient thermal structure of the atmosphere $T(z,t)$ over a period of days, usually in a valley.
2. Valley Winds. An episode can be compounded by the intensification of an inversion by cold drainage winds sliding underneath at night.
3. Lake Breezes. A large dammed river, such as the Ohio River, is essentially a lake. It is conceivable that a two-cell cylindrical circulation could develop on a clear day, with downflow in the middle and rising air on both shores, trapping pollutants in the circulation field.
4. Urban Thermal Circulation. This toroidal circulation, which is driven by the heat release of a city, can also trap and recirculate pollutants.

The authors have not yet brought these phenomena into a short-term model of such a city as Steubenville, Ohio.

"Urban Plume" Modeling for Ozone

The State of the Art of Ozone Modeling

Regression models for ozone as a function of some environmental variables, such as temperature and wind speed,[20,21] are available.

The diurnal curve of ozone concentration versus time is approximately a sinusoid plus a constant. This curve is the solution of the following differential equation:

$$\tau \frac{d[O_3]}{dt} = KI - [O_3]$$

where I is illumination intensity (a sinusoidal function of time) and where K and τ are constants. The authors have derived this equation from published sets of kinetic equations by making some reasonable simplifications.

The next most complicated model would take account of vertical movement (by diffusion or by transport in a lake breeze) and the vertical distribution of ozone over the diurnal cycle.[22] Then it would be desirable to model the growth and decay of ozone concentration in an urban plume extending into a rural area.[23] Until such models are available, further complication of the kinetics mocel seems unwarranted.

Considerations for Statewide Ozone Network

As a necessary preliminary to modeling ozone in Ohio, the monitoring network is being expanded. At present virtually all 28 monitors are urban. Hence it is desirable that all monitors added in the near future have rural sites. Each rural site should be within about 50 miles of at least one city and preferably at the centroid of several cities, in order that urban plumes can be studied.[22]

The Automotive Source Problem

Metropolitan Carbon Monoxide Modeling

All of this work has been done in cooperation with the Ohio Department of Transportation (ODOT). We initially thought to use the APRAC[24] model for this purpose. We approached ODOT to obtain the traffic-grid and vehicle load factors for the Columbus, Ohio area. It was quickly found that ODOT's number of traffic grid links exceeded the capacity of APRAC by about a factor of ten. Although an APRAC compatible grid for Columbus was eventually produced, it was concluded that such an approach was impractical for all Ohio cities.

A greatly simplified model called COPOLLUT[25] was developed for survey purposes. In the emission rate algorithm, only traffic links are assumed to produce the pollution pattern. Turning movements are not included. In the dispersion algorithm, wind direction is assumed to be at the same relative angle for each traffic link, and, therefore actual meteorological conditions are not used. Emission factors are taken from reference 28.

Thus the model emphasizes the emission characteristics of carbon monoxide pollution. Sophisticated dispersion relationships are not used. Such assumptions are compatible with measured concentration patterns[27] of carbon monoxide. The principal shortcoming of the model is its inability to handle the influence of street canyons upon dispersion. Such effects would be important, principally in the Central Business District. The model produces realistic patterns of pollution in the sense that they are neither largely better than nor worse than the air quality standards for Columbus.

Finite Line Source Model

A model described elsewhere in this conference[26] has been developed for modeling finite line sources. A closed-form, time-dependent solution has been derived. The dispersion function explicitly incorporates ground roughness and vertical heat flux. The incorporation of ground roughness and the functional form of the time dependence are thought to be quite characteristic of carbon moxoxide dispersion from roadways in a variety of areas of varying degrees of urban development. It is intended to be applied to analyses of proposed roadway development. It can also be readily adapted to Indirect Source complexes.

Conclusions

Our use of air quality models emphasizes their use for assessing environmental situations and for regulation development. We emphasize that models be theoretically realistic and hopefully simple. We further require them to be representative of the real world as attested by measurement comparisons.

Existing models which we have acquired deal with only an extremely limited number of real situations. Such models are restricted theoretically to flat terrain, steady-state, uniform wind, non-reactive pollutant situations. We are seeking and developing additional models which incorporate topography, kinetics, thermal structure (both vertical and horizontal), and diurnal phenomena such as valley winds, heat islands, and lake breeze.

The major air pollution problems in Ohio generally occur where some or all of these variables are present. We will not feel confident in defining the situation or devising control remedies until we can confidently model where and when these variables occur.

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DESIGNING A REGIONAL AIR POLLUTION MONITORING NETWORK: AN APPRAISAL OF A REGRESSION EXPERIMENTAL DESIGN APPROACH

P. R. Gribik
Graduate School of Industrial Administration
Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

J. R. Sweigart
School of Urban and Public Affairs
Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

K. O. Kortanek
Department of Mathematics
Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

ABSTRACT

The problem of allocating measuring resources to aid in accurately estimating ground level pollution concentrations throughout a region is examined. Application of optimal regression experimental design makes the uncertainty in the estimates small for a given measurement effort and suggests where the measurements should be taken. Design criteria are surveyed for this problem as well as the assumptions that underlie the application of this technique. The allocation and location problem is illustrated with a hypothetical example.

1. INTRODUCTION

Generally, the effectiveness of an air quality management program depends greatly upon the ability to estimate accurately the ambient air pollution levels throughout a given region. In turn, the ability to make accurate estimates depends upon the design of the monitoring network, specifically, upon the locations of the measuring equipment. In this paper we discuss the problem of allocating pollution measuring resources to satisfy the need for accurate estimation of the ground level concentration of a pollutant throughout a region. The techniques can be viewed as being source-oriented in that they give estimates of the pollution contribution of each source, which is important for use in an air quality management program. Results from a diffusion model are used to determine the form of a response surface with which one estimates the pollutant concentration at each point in the region, including those points where measurements are not made. Multivariate regression analysis can be used to fit the response surface to the measurements obtained from a monitoring network by computing numerical values of unknown parameters, such as the emission distribution of point sources. Before actually taking measurements and solving for these parameters, one first seeks to allocate the measurement resources to points throughout the region and thus determine sampling sites.

In this paper mathematical methods are surveyed which treat the problem of allocating these resources in some optimal way. The basic problem is one of regression experimental design, where the goal is to obtain good estimates of unknown parameters. Beginning with Section 2, the underlying experimental regression design model is presented. Basic assumptions are stated. In Section 3, design criteria are examined for the model which tend to make the uncertainty in the estimates of the parameters as small as possible in an economically efficient manner. The problem of resource allocation is treated under the assumption of a fixed weather state.

The basic assumptions introduced in Sections 2 and 3 are examined in Section 4. Finally, in Section 5 our conclusions are presented with a view towards implementation.

2. THE ESTIMATION OF UNKNOWN PARAMETERS: EMISSION RATES

Given a control region R, consider the problem of estimating the ground level concentration of a single pollutant throughout R by using measurements collected at a finite number of points in R. In R there are n known sources of pollutant and this pollutant is assumed not to react with any others. It is clear that pollution concentrations are highly dependent upon weather state as specified by wind direction, wind speed, mixing height, stability class and so forth. Consider a single weather state during which the need for accurate estimation of air pollution concentrations is acute.

For a particular weather state a diffusion model may be used to approximate the pollution concentration at any point x in R due to source i. This approximation is of the form $\theta_i u_i(x)$ where θ_i may be interpreted as the emission rate of source i and $u_i(x)$ is the pollution transfer function of the i^{th} source as determined by the diffusion model (with a unitary emission rate). Assuming unknown "background" pollution, θ_o, the pollution concentration at any point x in R can be written as

$$\theta_o + \sum_{i=1}^{n} \theta_i u_i(x). \tag{1}$$

In fitting (1) to actual measurements, linear regression analysis can be used to estimate

$\theta_o,\ldots,\theta_n$. Call these computed estimates $\hat{\theta}_o,\ldots,\hat{\theta}_n$. The resulting function

$$\hat{\theta}_o + \sum_{i=1}^{n} \hat{\theta}_i u_i(x)$$

is then used to estimate the concentration of pollutant at any point in R.

Assume that measurements of the pollutant are made at the points $x_1,\ldots,x_m$ in R with k_i measurements taken at x_i and that any observation can be written in the form,

$$\theta_o + \sum_{i=1}^{n} \theta_i u_i(x) + \epsilon(x). \qquad (2)$$

Here $\epsilon(x)$ is a random error term. Denote the result of the j^{th} measurement at x_i by g_{ij}, $j = 1,\ldots,k_i$ and set

$N = \sum_{i=1}^{m} k_i$ (the total number of measurements taken in R)

$M = \sum_{i=1}^{m} \frac{k_i}{N} u(x_i)u(x_i)^T$ (the information matrix for the given measurement scheme)

$b = \sum_{i=1}^{m} k_i u_i(x)\overline{g}_i$ and

$\overline{g}_i = \frac{1}{k_i} \sum_{j=1}^{k_i} g_{ij}$ (the average pollution reading at x_i for k_i measurements).

$u(x_i)$ is the column vector $(1,u_1(x_i),\ldots,u_n(x_i))^T$. If the information matrix M is non-singular, the least squares estimator of $\theta = (\theta_o,\theta_1,\ldots,\theta_n)^T$ is $\hat{\theta} = \frac{1}{N} M^{-1}b$. Since the total number of measurements that may be made in a period is fixed, the measurements should be allocated to points in R so that $\hat{\theta}$ is a good estimate of θ.

We consider the allocation problem under two standard assumptions that will be used in defining what is meant by $\hat{\theta}$ being a "good" estimate.

A1 The random errors in the observations are independent among all observations.

A2 The mean of $\epsilon(x)$ is 0 and the variance of $\epsilon(x)$ is λc where c is known while λ may be known or unknown.

Under these two assumptions, the covariance matrix of $\hat{\theta}$ is $(\lambda c/N)M^{-1}$. Since the covariance matrix of $\hat{\theta}$ gives an indication of the uncertainty in our estimates and we wish to make this uncertainty small in some sense, we consider the problem of allocating the measurement resources so as to "make the covariance matrix small" with respect to a particular criterion function. In the next section we discuss the allocation problem in more detail and the problem of choosing a criterion function.

3. THE PROBLEM OF ALLOCATING MEASUREMENT RESOURCES

The problem here is to determine the points in R where measurements are to be taken and the proportion of the total measurement effort to be expended at each location. Let $x_1,\ldots,x_m$ denote the points where measurements are to be taken and $p_1,\ldots,p_m$ denote the respective proportions. The problem here is not only to determine x_i and p_i but also the number of monitors, m. We define a design denoted by ϵ as follows:

$$\epsilon = \{(p_1,x_1),\ldots,(p_m,x_m)\}, \text{ where } \sum_{i=1}^{m} p_i = 1$$

and where ϵ is actually a function such that

$$\epsilon(x) = \begin{cases} 0 & \text{if } x \notin \{x_1,\ldots,x_m\} \\ p_i & \text{if } x = x_i \end{cases}$$

The problem can then be restated as one of finding a design which provides "good" estimates of pollution concentrations throughout R. As mentioned previously this can be done by making some function of the covariance matrix of $\hat{\theta}$, call it $\Phi(M)$, small. We thus propose the following non-linear optimization task, governed by a design criteria as specified by $\Phi(M)$.

Program P

Compute min $\Phi(M)$

for all $M \in R^{(n+1)\times(n+1)}$ and

$\{(p_1,x_1),\ldots,(p_m,x_m)\} \subset R^1 \times R$

subject to the constraints

$$M = \sum_{i=1}^{m} p_i u(x_i)u(x_i)^T$$

$$1 = \sum_{i=1}^{m} p_i$$

$$p_i \geq 0; \quad i = 1,\ldots,m$$

$$x_i \neq x_j \quad \text{for } i \neq j$$

and m is an arbitrary positive integer.

The solution to Program P, $\{(\hat{p}_1,\hat{x}_1),\ldots,(\hat{p}_m,\hat{x}_m)\}$, will be called an optimal design.

Another assumption is required.

A3 There is at least one design whose information matrix is non-singular for the given weather state.

Under assumptions A1-A3 the properties of Program P and its optimal designs will be examined for two design criteria. The functions that will be considered are

$-\log \det(M)$ and $\mathrm{tr}(GM^{-1})$ for some specified positive definite matrix G (det = determinate, tr = trace). The designs optimal for Program P under these two criteria are termed D-optimal and L-optimal designs, respectively. Fundamental contributions to the study of these problems have been made by Kiefer and Wolfowitz [8]. Mathematical properties of these problems and also some numerical algorithms for their solution are discussed in Fedorov [4].

Relying on a design$_n$ ϵ to estimate θ, the variance of $\hat{\theta}_o + \sum_{i=1} \hat{\theta}_i u_i(x)$ for any $x \in R$ is given by $\frac{\lambda c}{N} u(x)^T M^{-1}(\epsilon) u(x)$. $M^{-1}(\epsilon)$ denotes the inverse of the information matrix M which depends upon the design ϵ. Kiefer and Wolfowitz [8] have shown that a design ϵ^* is D-optimal if and only if its associated information matrix $M(\epsilon^*)$ solves

$$\min_{M \in \Omega} \max_{x \in R} u(x)^T M^{-1} u(x)$$

where

$$\Omega = \{M \in R^{(n+1)x(n+1)} \mid \text{there is a design } \epsilon \text{ for Program P such that } M = \sum_{x \in R} \epsilon(x) u(x) u(x)^T \text{ and } \det(M) \neq 0\}.$$

Thus the D-optimal design minimizes the maximum variance of the best linear unbiased estimates (BLUE) of ground level pollution concentrations in the region R.

The L-optimal design is related to the expected error in $\hat{\theta}$. Let θ_{true} be the vector of the true source strengths in equation (1). Since $\hat{\theta}$ is unbiased $E(\hat{\theta}) = \theta_{true}$ (E = Expected value operator). If the design ϵ is used to collect data during a given weather state, then

$$E[(\theta - \theta_{true})^T G(\theta - \theta_{true})] = \frac{\lambda c}{N} \mathrm{tr}[GM^{-1}(\epsilon)]. \tag{3}$$

Thus the L-optimal design problem is equivalent to finding the design for which the LHS of (3) is minimized. An important special case occurs when G is chosen to be the identity matrix. Then the L-optimal design seeks to minimize the expected sum squared of errors in the BLUE of θ.

Another important choice of G is

$$G = \int_R u(x) u^T(x) \delta(dx)$$

where δ is a probability measure on R for which G is non-singular. It can be shown in this case that the L-optimal design problem seeks to minimize the weighted average of the variance of the BLUE of the ground level pollutant concentrations in the region R where $\delta(\cdot)$ is the weighting term. One possible choice of $\delta(\cdot)$ is to set $\delta(A) = \frac{\text{pop A}}{\text{pop R}}$ where pop(A) = population of region A, for A some subset of R. In this case, Program P would determine an allocation that yields better estimates of the pollution in the more densely populated sections of R.

The final choice of the design criterion will depend upon the intended use of the estimated coefficients $\hat{\theta}_i$. If the estimated coefficients are to be used to estimate total concentration at points throughout R, any of the design criteria suggested is appropriate. However, if the purpose is to use the estimates of θ as estimated emission rates of sources to be used as a basis for regulatory policy, then the L-optimal design with $G = I$ should be taken.

4. DISCUSSION OF ASSUMPTIONS A1 THROUGH A3

The previous results depend upon the assumptions that were made. Assumption A1 is likely to be difficult to satisfy and deserves further discussion. This assumption depends upon the accuracy of the diffusion model and the interpretation and implementation of the optimal design. Suppose that we use one of the previous models and obtain $\{(p_1^*, x_1^*), \ldots, (p_m^*, x_m^*)\}$ as an optimal design. Also suppose that we are to take N measurements and that we interpret the optimal design to mean that we are to take $p_i^* N$ observations at x_i^* with all measurements taken at the same time. Under this interpretation, the assumption that the deviations of the measurements from the model are independent (A1) may well be violated. For assumption A1 to be valid under this interpretation, we would need a diffusion model that was accurate down to very small scale effects. Since the diffusion models available at present are not this accurate, this interpretation is not adequate.

Assume that the diffusion model used can accurately model effects as small as d meters in diameter and t minutes in duration. Let

$$T = t \cdot (\max_{i \in \{1, \ldots, m\}} p_i^* N)$$

and assume that the weather state remains unchanged and that the emission rates of the sources and other parameters of the point sources remain constant for a period of T minutes. If we take a measurement at point x_i^* every $T/(p_i^* N)$ minutes during this period of T minutes and if $\min_{i \neq j} \|x_i^* - x_j^*\| \geq d$ where $\|\cdot\|$ is the Euclidean norm on R^2, then the deviations of the measurements from the model will be independent.

If $\min_{i \neq j} \|x_i^* - x_j^*\| < d$, we can alter the previous programs to insure that the points in a design are far enough apart. One way would be to add the constraints

$$\|x_i - x_j\| \geq d \quad \text{for} \quad i \neq j$$

to a program. However these constraints are nonconvex and so increase the difficulty of solving the program. There is another way to insure that $\min_{i \neq j} \|x_i^* - x_j^*\| \geq d$ which is consistent with the practicalities of the problem.

In a practical problem, the optimal design would probably not be exactly implemented but only used as a guide since factors not precisely modeled would also be considered. For example, a monitoring station would not be placed in the lee of a large building or next to a minor pollution source that was only considered in the aggregate background pollution θ_o. Hence, if a sufficiently fine grid H on R is chosen, the resulting optimal design would be adequate for our purposes.

If the grid H satisfies

$$\min_{\substack{x,y \in H \\ x \neq y}} \|x - y\| \geq d \qquad (4)$$

then no two points in an optimal design can be closer than d and so assumption A1 will be satisfied. In U.S. regional air pollution studies, grid squares are typically one to ten kilometers on a side. If the region R is such that $\max_{x,y \in R} \|x - y\| \gg 10$ kilometers, which is the case in most problems of interest, and if d is on the order of one to ten kilometers or smaller, H can be chosen to be a grid sufficiently fine to yield useful results while satisfying (4). Also, a grid H will insure that no further assumptions on the transfer functions and the region R are needed.

5. CONCLUSIONS: INTERPRETATIONS AND IMPLEMENTATION

The previous models consider the problem of allocating measurement resources to collect pollution concentration data during the time that a specified weather state holds. Since the optimal allocation depends upon the transfer functions obtained from a diffusion model and these functions depend upon the weather state, the models developed may give different optimal allocations for different weather states. We do not suggest proportionally dividing the equipment among the allocations optimal for the different weather states since the result may not be a good allocation to the overall problem.

One way to approach this problem is to extend the methods of this paper to more than one weather state. In this case, it is necessary to choose a set of weather states $S = \{s_1, \ldots, s_k\}$ which is of interest. We then wish to design a monitoring network for the region R so that good estimates of the parameters θ_i can be made, on the average, when the weather state is in the set S. Let w be a random variable which denotes the weather state at some time in the future where frequency data can be used to estimate the conditional probability that w is in S. The details of this extension have been completed in P. R. Gribik's Thesis [6].

The methods of this paper are directly applicable if one is willing to choose a prevailing or typical weather condition for the region and design on it. Another direct approach would require the utilization of a long-term diffusion model and a prespecified frequency distribution on wind direction and wind speed. Then, the measurements would be used to develop long-term averages at the given set of design points and the p_i would be interpreted as the proportion of measurement effort to be expended at point x_i to develop this average. The main use of the estimated parameters computed in this situation would be for the calibration of the diffusion model results.

It is highly desirable that a regional monitoring network provide information on air quality both in the short-run and the long-run. The above alternatives suggest a variety of ways in which this goal may be accomplished. For example, a monitoring network which is for all practical purposes stationary, can be established to satisfy the needs for long term estimation. If this network is not satisfactory in the short-run it would be necessary to determine a set of "critical" weather states where the probability of exceeding ambient air quality standards is high. For critical states designs could be computed and for short periods of time during these critical states mobile monitoring equipment could be placed at the previously designated locations.

The methods described in the paper are perhaps more attractive if mobile monitoring equipment is available, but the application of the methods is still reasonable if all equipment is stationary. The actual implementation plan will of course depend upon the resources available as well as individual characteristics of the region under consideration.

6. AN ILLUSTRATION OF THE ALLOCATION PROCEDURE

In this section we consider a small example which illustrates the allocation procedure and indicates a sample allocation of resources. Suppose we have a region with four major polluters and an unknown background source. The four sources are described as follows:

Source #	HP (m)	TS (deg K)	VS (m/sec)	D (m)	VF (m^3/sec)	R (mi)	S (mi)
1	61.0	600.	6.1	2.6	32.4	5.7	3.9
2	34.7	727.	1.6	1.5	2.8	6.5	4.7
3	113.0	546.	9.3	5.2	197.5	2.9	5.7
4	50.0	460.	7.0	2.5	34.4	7.0	2.9

and

HP: physical stack height
TS: stack gas temperature
VS: stack gas exit velocity
D: inside diameter of stack
VF: stack gas volumetric flow rate
R: x-coordinate of stack
S: y-coordinate of stack.

The EPA computer program DBT51 which calculates concentrations for multiple point sources was used to calculate concentrations at 729 grid points (1 mile grid) for a single weather state. A typical weather state was defined by Pasquill's stability class D, wind speed - 5 m/sec, mixing lid - 1219 m, ambient air temperature - 284 deg K, and with wind from the southwest. For purposes of illustration we choose a non-uniform grid of 80 points which reflect the changes in individual contributions of the sources involved. Figure 1 indicates the diffusion coefficients × 100 at the 80 points considered. The locations of the sources are also indicated in Figure 1. For each of those locations contributions from each of these sources are computed and stored.

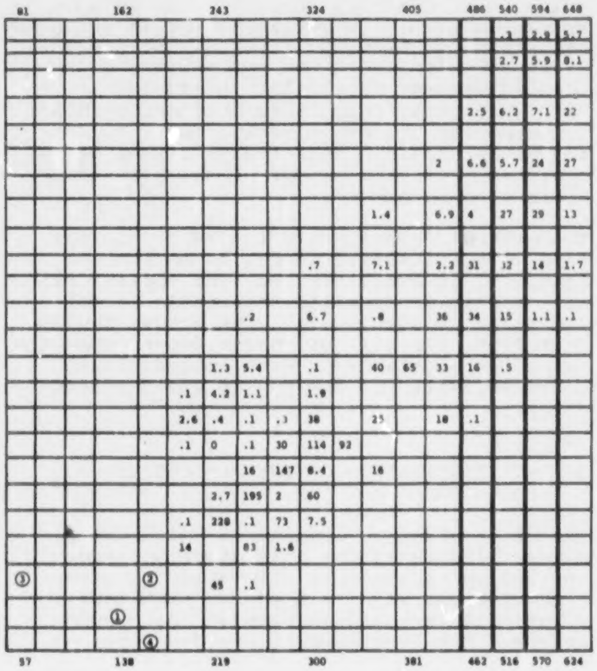

Figure 1: Total concentrations at 80 locations in R

Let us choose our design criteria as the one which minimizes the maximum variance of the best linear unbiased extimate (BLUE) of ground level pollution over the chosen grid, i.e., we propose to compute a D-optimal design. Using an algorithm proposed by Fedorov [4] (p. 102) we specify an initial design and proceed to obtain a solution to Program P. The initial design as well as an "approximate optimal design" are given below.

Initial Design

Location (grid point #)	223	226	251	305	368
Mass (p_i)	.2	.2	.2	.2	.2

Final Design

Location (grid point #)	223	226	251	305	368	307	249
Mass (p_i)	.195	.198	.009	.009	.199	.196	.194

Even without termination it appears that a design is emerging with monitors at grid points 223, 226, 368, 307, and 249 and with approximately the same measurement effort to be expended at each of these points. It is informative to note the individual contributions of the sources at each of these locations.

Monitor #	Location	Sources #1	#2	#3	#4
1	223	46.62	181.64	0	0
2	226	0	0	0	0
3	249	0	0	0	82.3
4	307	39.4	74.46	0	0
5	368	0	0	7.07	0

In this problem it can be projected that 1 and 4 monitor sources 1 and 2, 2 monitors the background pollution, 3 monitors source 4, and 5 monitors source 3. We also note that an initial design with points 196, 202, 335, 424, and 648 led to a comparable outcome. The implication to the estimation problem goes as follows. Locate monitors at 223, 226, 249, 307, and 368 and take approximately the same number of measurements at each location during the weather state specified. Use the average of these measurements, $\bar{g}_1,\ldots,\bar{g}_5$ to fit the measurements to the diffusion model estimates and then use $\hat{\theta}_o + \sum_{i=1}^{4} \hat{\theta}_i u_i(x)$ to estimate concentrations at the remaining 75 grid points. We can then guarantee that these estimates are "best" in the sense described earlier in this section.

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SAMPLED CHRONOLOGICAL INPUT MODEL (SCIM) APPLIED TO AIR QUALITY PLANNING IN TWO LARGE METROPOLITAN AREAS

R.C. Koch, D.J. Pelton and P.H. Hwang

GEOMET, Incorporated
Gaithersburg, Maryland

Summary

SCIM is a multiple-source urban diffusion model based on the Gaussian plume equation and has been used to analyze SO_2 control regulations in Boston and San Francisco. Maximum 3-hour, 24-hour, and annual mean concentrations are calculated from NEDS emission or fuel use data and standard National Climatic Center data. Model validation results for Boston show a model to measurement correlation of 0.97 for annual means and 0.81 for maximum 24-hour concentrations of SO_2 based on comparisons at 14 stations. The analysis showed that fuel regulations which permit increasing fuel-sulfur to 1 percent in the Boston core area will not meet National Ambient Air Quality Standards (NAAQS). In San Francisco the analysis showed that limiting SO_2 emissions from large sources is more critical for meeting NAAQS than is limiting the sulfur content of fuels.

Introduction

Projected shortages of low-sulfur fuels have caused many states to reexamine their regulations for controlling sulfur emissions. Areas where present regulations are more stringent than necessary to meet air quality standards may be suitable for more lenient SO_2 emission regulations. Proper evaluation of this question in large metropolitan areas, which contain large power plants and chemical processing plants and where substantial quantities of fuel are used for space heating, requires the use of a computer simulation model to account for the effects of many sources and to determine both the long-term and maximum short-term air quality levels resulting from these sources. The recent requirement to develop air quality maintenance plans for many urban areas also requires the use of a dispersion model capable of evaluating air quality levels from many simultaneous sources. The multiple-source Gaussian plume dispersion model can be used to make these evaluations. This paper describes the application of such a model, the Sampled Chronological Input Model (SCIM), to evaluate alternative SO_2 control strategies in Boston and San Francisco.

Model Description

SCIM is based on the Gaussian plume equation with the origin at a receptor point of interest and the x-axis pointed upwind into the mean wind direction. Assuming an impervious ground surface and an exponential depletion constant (k) to account for physical and chemical removal processes, the ground-level concentration from a point source is given by:

$$\chi = \frac{q}{\pi \mu \sigma_y \sigma_z} \exp\left\{-\frac{y^2}{2\sigma_y^2} - \frac{kx}{\mu} - \frac{h^2}{2\sigma_z^2}\right\}$$

Let q(dx)(dy) be the total amount of pollutant emitted per unit time in a horizontal element of area (dx)(dy). Assuming that the total concentration at a receptor is the sum of concentration contributions from all individual area source elements with an effective area source height h_A, the concentration χ_A at the receptor location due to the area source is:

$$\chi_A = \int_0^{x_1}\int_{y_1}^{y_2} \frac{q}{\pi \mu \sigma_y \sigma_z} \exp\left\{-\frac{y^2}{2\sigma_y^2} - \frac{h_A^2}{2\sigma_z^2} - \frac{kx}{\mu}\right\} dy\, dx$$

The integration operation is simplified by the "narrow plume" assumption, that:

$$\frac{1}{\sigma_y} \int_{y_1}^{y_2} q \exp\left\{-1/2\left(\frac{y}{\sigma_y}\right)^2\right\} dy = \sqrt{2\pi}\, \bar{q}(x)$$

As long as the spatial distances between variations in area-source emission rate are large compared to the horizontal diffusion parameter, it may be assumed that:

$$\bar{q}\,(x) \approx q(x,o)$$

As a result,

$$\chi_A = \sqrt{\frac{2}{\pi}} \int_0^x \frac{\bar{q}(x)}{\mu \sigma_z} \exp\left\{-1/2\left[\frac{h}{\sigma_z}\right]^2 - \frac{kx}{\mu}\right\} dx$$

This equation is evaluated using a variation of the trapezoid rule in which small increments in x are gradually increased with increasing x to a uniform increment. Area sources may be defined for up to five area source heights.

The effects of the two types of sources (area and point) are analyzed separately and added together to give a resultant concentration.

Limited Mixing

The marked reduction in vertical diffusion which is caused by a stable layer aloft is approximated using a suggestion by Pasquill (1962) that a uniform vertical distribution will be approximately achieved at a downwind distance from the source at which σ_z is equal to the height of the mixing layer. At half this height no effect due to limited mixing needs to be considered. Using linear interpolation between these distances and assuming σ_z is represented as a simple power law of x:

$$\sigma_z(x) = bx^q,\ x \leq x_1$$

$$\sigma_z(x) = L,\ x \geq x_2$$

$$\sigma_z(x) = \frac{L}{2}\left[1 + \left(\frac{x - x_1}{x_2 - x_1}\right)\right]\ x_1 < x < x_2$$

$$x_1 = \left(\frac{L}{2b}\right)^{\frac{1}{q}},\ x_2 = \left(\frac{L}{b}\right)^{\frac{1}{q}}$$

Plume Rise

The effective height of point sources is represented as the stack height plus a plume rise calculated using Briggs (1969) equations for leveled off plume heights. For stable conditions (Pasquill stability class E) assuming a potential temperature gradient of 0.02°c/m:

$$\Delta H = 2.9 \left(\frac{F\ T_a}{0.03034\ u} \right)^{0.33}$$

$$F = 2.45 \left[1 - \left(\frac{T_a}{T_s} \right) \right] V_s D_s^2$$

For neutral and unstable conditions (Pasquill stability classes A through D):

$$\Delta H = \frac{3.75 F^{0.33} X^{0.67}}{u}$$

$$X = \begin{cases} 2.16 F^{0.4} H_s^{0.6} & , H_s \leq 305 \\ 67.3 F^{0.4} & , H_s \geq 305 \end{cases}$$

Wind Speed

The wind speed is estimated for each effective point or area source height using the following power law (e.g., Munn 1966):

$$\mu(h) = \mu_1 \left(\frac{h}{h_1} \right)^a$$

Three values of "a" are input to SCIM corresponding to unstable (classes A, B, and C), neutral (class D) and stable (classes E and F) conditions.

Diffusion Parameters

Diffusion parameter values either for rural conditions (Pasquill 1962) or for urban conditions (McElroy and Pooler 1968) are used to characterize σ_y and σ_z by power law functions.

$$\sigma_y = ax^p$$

$$\sigma_z = bx^q$$

The rural parameters are given in Table 1, and the urban parameters are given in Table 2.

Table 1. Fitted Constants for the Pasquill Diffusion Parameters

Stability Class	Crosswind Constant(1)	Constants for Vertical Diffusion Parameter, σ_z(2)							
		$x \leq x_1$		x_1	$x_1 \leq x \leq x_2$		x_2	$x_2 \leq x$	
	a	b	q	(Meters)	b	q	(Meters)	b	q
A	0.40	0.125	1.03	250	0.00883	1.51	500	0.000226	2.10
B	0.295	0.119	0.986	1000	0.0579	1.09	10,000	0.0579	1.09
C	0.20	0.111	0.911	1000	0.111	0.911	10,000	0.111	0.911
D	0.13	0.105	0.827	1000	0.392	0.636	10,000	0.948	0.540
E	0.098	0.100	0.778	1000	0.373	0.587	10,000	2.85	0.366

(1) $\sigma_y = ax^{0.903}$, where x is downwind distance from the source; σ_y and x are in meters.

(2) $\sigma_z = bx^q$; σ_z and x are in meters.

Table 2. Fitted Constants for Urban Parameters Based on Turner Stability Classifications

Stability Index	Crosswind Constants (1)		Constants for Vertical Diffusion Parameter (2)			
			$x \leq 600$		$x \geq 600$	
	a	p	b	q	b	q
A(3)	-	-	-	-	-	-
B	1.42	0.745	0.0926	1.18	0.0720	1.22
C	1.26	0.730	0.0491	1.11	0.169	1.01
D	1.13	0.710	0.0835	1.08	1.07	0.682
E	0.998	0.650	0.0777	0.955	1.01	0.554

(1) $\sigma_y = ax^p$, where x is downwind distance from source; σ_y and x are in meters.
(2) $\sigma_z = bx^q$; σ_z and x are in meters.
(3) Not available from McElroy and Pooler data; use Class B values.

The stability classification used in SCIM is based on the Pasquill classes of atmospheric stability using a system suggested by Turner (1964). The Turner stability categories are determined from routine airport weather observations.

Mixing Height

The procedure which is used to define the height of the mixing layer is the following: Determine the vertical temperature profile from the nearest appropriate (same air mass) radiosonde, or by interpolation of two or more nearby radiosondes. Estimate minimum morning and maximum afternoon air temperatures which are representative of the urban area. The afternoon temperature may be obtained directly from airport observations or other available data. In most cases the morning urban temperature will exceed the rural temperature. Construct adiabatic temperature profiles from the urban temperatures which intersect the rural temperature profile. The heights of these intersections are assumed to be the minimum and maximum mixing heights. The method of interpolating between these values to give hourly estimates is:

1. Use the morning minimum from midnight to 6 a.m.

2. Linearly interpolate between the minimum and maximum between 6 a.m. and 2 p.m.

3. Use the afternoon maximum between 2 p.m. and midnight.

Validation

Validation in San Francisco

The average ratio of predicted to observed 20-day mean concentration for 20 stations is 1.0, which is an excellent agreement. The ratios obtained for each of three regions are more instructive.

The Martinez (northeast) and Richmond (north) regions are the areas of most interest since most of the large sources are located in those regions. In the Richmond region the model tends to overpredict the concentration and the regional average ratio is 1.4. In the Martinez region the station to station ratios are more uniform than in the Richmond region, however the regional average predicted to observed ratio is 0.4, which is not quite as good in the Richmond region. There is a consistent and general underprediction in the Martinez region but the ratios are fairly uniform. Validation results were not as favorable in the San Francisco region where the predicted to observed ratio is 3.9. Because the observed concentrations in this area were consistently below the sensing threshold of the monitors, no particular significance is attached to this result. Overall, the performance of the model on the 24-hour average SO_2 concentrations from 20 stations for a 20-day sample was judged to be acceptable.

Validation in Boston

Annual Means. SO_2 concentrations measured using gas bubblers were compared to model calculations based on 8 hourly calculations, one for every third hour of the measurement day (Koch, 1975). The calculated values generally exceeded the measured values by a small amount varying from about 5 $\mu g/m^3$ when the measured value is 10 $\mu g/m^3$ to about 7 $\mu g/m^3$ when the measured value is 50 $\mu g/m^3$. The correlation coefficient for the 15 pairs of values is 0.97.

Maximum 24-Hour Concentration. SO_2 concentrations were calculated for all days for which a measurement was available for 1972. The maximum measured and calculated values do not necessarily correspond to the same day. The calculated values deviate from the measured value by a maximum of 50 $\mu g/m^3$ for a measured value of 150 $\mu g/m^3$ and by 35 $\mu g/m^3$ for a measured value of 75 $\mu g/m^3$. The correlation coefficient is 0.81 for the 14 values for which comparisons were made. The mean difference of measured minus calculated concentration is 2.4 $\mu g/m^3$, and the standard deviation of the differences is 26 $\mu g/m^3$.

Maximum 3-Hour Concentration. Hourly concentrations of SO_2 were measured at four monitoring sites. Calculations were made for every third hour for days on which concentrations were measured. Three of the four calculated maximums are within 10 percent of the maximum measured values. At one site the calculated value exceeded the measured value by 50 percent. However, since the calculations for two of the sites are suspected to be subject to errors in the emission inventory, these results are not conclusive regarding the model validity in estimating maximum 3-hour concentrations.

Distribution of 24-Hour Concentrations. The characteristics of the frequency distribution of paired, measured, and calculated 24-hour concentrations at 14 stations were determined (see Table 3).

Table 3. Summary of Correlations Between Parameters of Paired, Measured, and Calculated 24-Hour SO_2 Concentrations

	Correlation Coefficients
Distribution Characteristics	14 Monitoring Sites
Maximum Value	0.81
95th Percentile	0.89
Mean	0.97
Geometric Mean	0.97
Standard Deviation	0.89
Geometric Standard Deviation	0.21

The measured and calculated values were sorted and ranked from high to low value, independently, and the percentiles were determined by linear interpolation of the ranked arrays. The paired percentile values do not necessarily correspond to any specific day.

The measured distribution is well represented by the model calculations, although the individual day-to-day comparisons are not as well correlated as the ranked percentiles might lead one to expect. The correlation coefficients for calculated and measured values at a single station vary from 0 to 0.6 and average about 0.3.

The chief reasons why day-to-day variations in SO_2 concentrations are not simulated in chronological sequence are:

- Only annual fuel consumption by point sources is accurately estimated. Seasonal, weekly, and daily variations are not represented.
- The allocation of residual and distillate oil to area sources is only an approximation.
- While temperature is the best known basis for estimating variations in fuel consumption for space heating, the sensitivity of different fuel users is not well known.
- Meteorological data obtained from a single site may not be representative of a metropolitan-area-wide average on some days.

The uncertainties cited above have plagued all urban modeling studies. The result is that, over a significant period of time (a year or more) the average concentrations on a given day may vary significantly from the model estimate. This is due to randomly distributed errors balancing out over a long period of time.

Evaluation of Alternative Fuel-Sulfur Regulations in the Boston AQCR

The SCIM model was used to analyze the impact of eight fuel scenarios (described in Table 4) on the ambient concentrations of SO_2 in the Metropolitan Boston area. Sulfur dioxide concentrations were calculated for every third hour of every sixth day of 1972 at 135 receptor locations (Koch, 1975).

Table 4. Fuel Sulfur Content for Boston AQCR Fuel Regulation Strategies

	Maximum Fuel Sulfur Content (Percent)		
		Residual Oil and Coal	
Strategy Number	Distillate Oil	Boston Core Area*	Outside Core Area
1	0.3	0.5	1.0
2	0.3	1.0	1.0
3	0.3	0.5	2.0
4	0.3	1.0	2.0
5	0.5	0.5	1.0
6	0.5	1.0	1.0
7	0.5	0.5	2.0
8	0.5	1.0	2.0

* Core area consists of 13 towns, including Arlington, Belmont, Boston, Brookline, Cambridge, Chelsea, Everett, Malden, Medford, Newton, Sommerville, Waltham and Watertown.

Emission Inventory

Sulfur dioxide emissions for point and area sources were estimated from the 1972 state emission inventory which included sulfur dioxide emissions, amount and type of fuel used, and data related to the effective height of emissions for 356 point sources and 1718 area sources.

The point source data were used without attempting to account for seasonal or diurnal variations in the rate of sulfur dioxide emissions. Area source emissions which have a greater impact on ground-level concentrations than point sources, because they are released at lower heights and have less buoyancy, are mostly due to space heating. It is reasonable to generalize on the seasonal and diurnal variations in their emissions using the relationship:

$$\frac{Q_i}{Q_t} = (1 - F) + \frac{FD_i}{S} (H_i - T_i)$$

$$S = \sum D_i (H_i - T_i), \text{ annual sum.}$$

The parameters D_i and H_i (Table 5) were previously determined by the best fit between model calculations and sulfur dioxide measurements in New York City. A value for F (the fraction of emissions which are sensitive to temperature) of 0.8 was adopted for the Boston area based on correlations between model calculations using experimental values of F and sulfur dioxide measurements at some 20 sites.*

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*It was later reported to M. Rosenstein of EPA Region I by the Better Home Heating Council that 85 percent of fuel usage by a typical Boston home is for space heating.

Table 5. Hourly Values of Fuel Demand Parameters for Estimating Space Heating

Hour of the Day	H: Heating Threshold Temperature (°F)	D: Peak Demand Factor
1	55	0.328
2	55	0.329
3	55	0.341
4	56	0.434
5	58	0.840
6	59	1.416
7	61	1.686
8	63	1.423
9	64	1.145
10	65	1.044
11	65	0.988
12	65	0.986
13	65	0.998
14	65	1.003
15	65	1.039
16	65	1.182
17	65	1.243
18	65	1.313
19	65	1.339
20	65	1.306
21	64	1.200
22	62	0.816
23	60	0.487
24	58	0.386

The five meteorological parameters required as input to SCIM are: (1) wind direction, (2) wind speed, (3) temperature, (4) atmospheric stability, and (5) mixing height. Measurements of wind speed and direction, cloud cover, and air temperature observed at Logan Airport in Boston every third hour of the day during 1972 were obtained on magnetic tape from the National Climatic Center (NCC) in Asheville, North Carolina. The wind speed, total amount of cloud cover in tenths, and the height of the cloud ceiling were used in the SCIM model to determine the atmospheric stability class. A special program was used to calculate the mixing height for each 12-hour radiosonde observation time using the radiosonde data for Portland, Maine, and the surface temperature observed at Logan Airport. The mixing height is defined as the greatest height to which a parcel of air at the surface can be lifted before it becomes 1°C or more colder than atmospheric temperatures as indicated by the radiosonde temperature profile. Temperature changes in the displaced parcel are computed assuming adiabatic expansion of the air and adsorption of any latent heat due to condensation as the parcel is lifted. The 12-hour mixing heights are interpolated to hourly values.

Annual Mean Concentrations of SO_2

The annual mean concentrations computed by the model show that the highest concentrations for each scenario occur in three locations which form a belt stretching from South Boston through the Boston Hub to Everett. This belt runs through the center of the principal sources of SO_2 as shown in Figure 1.

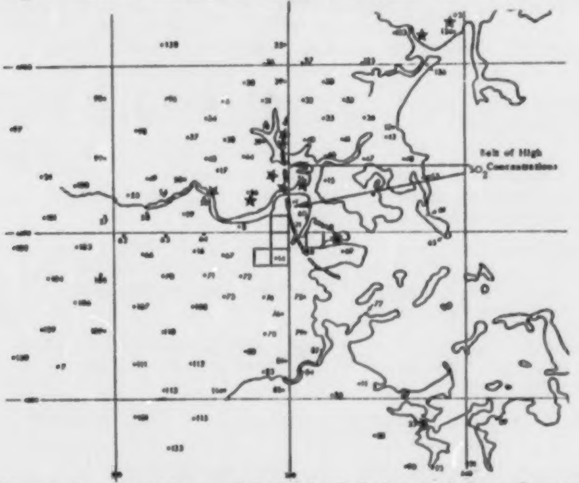

Figure 1. Locations of Principal Point and Area Sources of SO_2, Belt of High Computed SO_2 Concentrations, and Receptors Used for Model Calculations

Key:
★ Point Source (>10g/sec)
□ Area Source (>5µg/m^2/sec)

The primary National Ambient Air Quality Standard for annual mean concentrations of SO_2 (80 µg/m^3) is exceeded in the belt of high concentrations in scenarios 2, 4, 6, and 8. These are the scenarios in which fuels other than distillate oil are allowed to contain 1.0 percent sulfur in the Boston core area. Furthermore, the gradient around the high belt zone is intensified as compared to the present situation (scenario 1). In scenarios 3, 5, and 7 the increases are much more uniform and dispersed. In scenario 7, in which both the sulfur content of all distillate oil and the sulfur content of other fuels outside the core area are raised, the maximum concentration in the belt zone is very close to the NAAQS.

Maximun Short-Term Concentrations of SO_2

The calculations for each receptor were used, assuming a log-normal distribution, to estimate the 99.73 percentile (i.e., 364/365 of the distribution) and the 99.97 percentile (i.e., 2919/2920 of the distribution), respectively. The geometric mean and standard deviation for 24-hour values were determined from the average of eight 3-hour values for every sixth day. All values were used to determine a geometric mean and standard deviation of 1-hour values. The 1-hour and 24-hour values were converted to 3-hour values using the relationships suggested by Larsen (1971). The minimum of the two estimates was selected.

The percentile values were determined as follows:

$$C_p = m_g (s_g)^{Z_p}$$

Using this procedure, the 24-hour NAAQS was found to be exceeded at several locations for every scenario. The distribution of calculated 24-hour concentrations was plotted on log-probability scales for each location which exceeded the NAAQS and for sufficient additional locations to identify the maximum concentration associated with each scenario. At most of the locations examined, it was found that the distribution leveled off near the high values and the calculated log-normal distribution was a poor fit. However, the high end of the distribution could be fitted by eye to a straight line which was consistent with the data. An extrapolation of this visually fitted line was used to derive a new, more reasonable estimate of the concentrations not exceeded more than once per year.

When the top part of the distribution is extrapolated graphically to determine the annual maximum concentration, it is estimated that for scenarios 1, 3, 5, and 7 none of the sites will exceed the 24-hour standard. When this procedure is repeated for 3-hour concentrations, it is estimated that for scenarios 1, 3, 5, and 7 none of the sites will exceed the 3-hour standard. With regard to the scenarios 2, 4, 6, and 8, it is estimated that both the 3-hour and 24-hour standards will be exceeded at several locations due to the potentially large increase of SO_2 emissions from point sources in the core area.

Table 6. Maximum Concentrations For Each Scenario

Scenario	Annual		24-Hour		3-Hour	
	Receptor	Concentration (µg/m^3)	Receptor	Concentration (µg/m^3)	Receptor	Concentration (µg/m^3)
1	69	60	69	260	40	800
2	69	110	69	500	40	1500
3	1, 69	60	10, 93	290	40	800
4	69	110	69	500	40	1500
5	69	65	74	290	40	800
6	69	115	69	500	40	1500
7	1	70	10	330	10	860
8	69	115	76	510	40	1500

Evaluation of Alternative SO_2 Emission Limitations in San Francisco

The impact of control strategies which limit process source emissions to no greater than 300, 500, 1000, or 2000 ppm or which limit the sulfur content of the fuel in combustion sources to 0.3, 0.5, 0.7, and 0.9 percent sulfur were evaluated for the San Francisco Bay Area. As a further consideration, an alternative to limit power-generating plants to consumption of 0.5 percent sulfur fuel oil and prohibit their use of natural gas was evaluated. These nine alternatives, plus the present emission situation, form the ten strategies evaluated in this study.

Source Emission Inventory

Data were obtained for point and area sources from the Bay Area Air Pollution Control District (BAAPCD). The data for 41 points were updated by reviewing several sets of supplementary data to select those which are complete and are most representative. No seasonal or diurnal variations were applied to the point source emissions. The area source emissions were represented by uniform 5 km squares over the whole area. Seasonal and diurnal variations in emissions were furnished by BAAPCD for each grid square.

Meteorolgical Data

Meteorological data used in this study included surface observations from San Francisco and Oakland International Airports, upper air observations from Oakland International Airport, and surface wind speed and direction from seven sites operated by private companies. A vector average of wind speed and direction was computed for each of three regions, which provides a reasonable spatial variation of the wind throughout the area.

Analysis

Monthly variations in the power plant emissions and hourly variations of the area source emissions were represented in the model. Due to the complex wind patterns in the Bay Area three separate regions representing meteorological and geographical groupings of the SO_2 sources were used. Winds for each source region are used to advect SO_2 into neighboring regions. 24-hour average concentrations were made for every other day in 1973 by averaging eight 1-hour concentrations.

The annual mean and the highest predicted 24-hour average concentration for each of the ten strategies were determined for each of 120 locations based on hourly evaluations for about 1300 hours. The annual maximum 24-hour concentration was estimated by statistical extrapolation of the geometric mean and the geometric standard deviation, assuming a log-normal distribution.

It was found that the national standard for annual means is not exceeded at any point under all ten of the strategies. However, the 24-hour standard will be exceeded if a strategy is developed which allows non-combustion emissions of SO_2 which exceed 2500 ppm. Based on this finding, it is recommended that both a concentration-emission limit for process industries (e.g., 2000 ppm) and a fuel-sulfur limit (e.g., 1.0 percent) be adopted for the Bay Area.

Symbols

a, b, p, q - Empirical parameters for diffusion functions (σ_y and σ_z)

C_p, χ, χ_A - Concentration

q - Point source emission rate

Q_i, Q_t - Area source emission rate per unit area

D_i, H_i - Space heat demand factor and temperature threshold

F - Fraction of emissions due to space heating

D_s, H_s, T_s, V_s - Stack diameter, height, temperature, and velocity

h, h_A - Effective stack height

ΔH - Plume rise

μ (or μ_1) - Wind speed (μ_1 means height h_1)

k - Exponential pollutant decay constant

L - Mixing height

m_g, s_g - Geometric mean and standard deviation

x, y - Alongwind and crosswind rectangular coordinates

x_1, y_1, y_2 - Distances to upwind and crosswind edges of area source

T - Air temperature

σ_y, σ_z - Horizontal and vertical diffusion parameters.

Z_p - Standard deviation corresponding to percentile p

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MODELING OF PARTICULATE AND SULFUR DIOXIDE IN SUPPORT OF TEN-YEAR PLANNING

Richard A. Porter, P.E.
Meteorology
Texas Air Control Board
Austin, Texas

John H. Christiansen
Data Processing
Texas Air Control Board
Austin, Texas

Summary

Urban air pollution modeling is a vital part of the planning for attainment and maintenance of ambient air quality standards. A Gaussian plume model based on annual climatology and an accurate emissions inventory can be made to represent adequately the ambient conditions in an urban area through calibration with ambient air quality data. A model such as the Texas Climatological Model that incorporates options for use in control strategy development allows the analyst to identify sources of current and projected violations of ambient air quality standards.

Introduction

Mathematical modeling is an important tool for relating emitted pollutants to ambient air quality for air quality maintenance planning and analysis. As such, there are three important elements in the modeling process: emissions inventory, the computer model algorithm, and air quality data from ambient air monitors. This paper discusses the modeling process as it applies to support for Air Quality Maintenance Planning and Analysis (AQMPA) for the pollutants sulfur dioxide (SO_2) and total suspended particulate (TSP). A method of obtaining and maintaining an emissions inventory for modeling is discussed. The Texas Climatological Model (TCM) computer algorithm and its use is outlined. The use of ambient air quality data for model calibration is illustrated. Finally, model projections of ambient air quality for future years are discussed.

Emissions Inventory

The emissions inventory for Air Quality Maintenance Planning and Analysis (AQMPA) modeling is divided into emission from point sources and emissions from area sources. For a typical Gaussian plume model, the information required for point sources is location, emission rate, and stack parameters (stack height, stack diameter, exit gas flow rate, and exit gas temperature). Area sources are formed as squares of various sizes. The information required for area sources is location of the southwest corner, length of a side of the square, and the emission rate. Point sources are usually the major sources of pollution; therefore, a major effort should be made to be as accurate and detailed in the point source inventory as possible. Area sources are appropriate for aggregating the relatively small numerous sources such as residential space heating and vehicle traffic. Guidance for establishing emission inventories is provided by the Environmental Protection Agency (EPA).[9]

In a major urban area the cost of gathering a special one-time emissions inventory is prohibitive. Fortunately the information gathered by the states for the National Emissions Data System (NEDS) can be processed to provide a point source emissions inventory for modeling; however, such data are not available as one of the regular reports from NEDS. Once an inventory base has been established, it is desirable to establish a system for updating the inventory so that in successive years a current inventory will be available for modeling. The Texas Air Control Board has devised a method of inventory maintenance that combines the use of annual inventory of specified industrial sources with onsite inspection and permit monitoring to continually update the emission inventory. A base year emissions inventory for 1973 was established by mailing questionaires to all known major sources of pollution. In future years questionaires will be mailed to all accounts that have more than 500 tons/year emissions of any pollutant. In addition, inventories will be updated any time an operating permit application is approved for new or expanded facilities; and all visits to facilities by investigators from the State or Regional offices of the Texas Air Control Board will include a check for changes to the emissions inventory for that account.

Computer Dispersion Algorithm

The primary computer algorithm used for AQMPA planning by the Texas Air Control Board is the Texas Climatological Model (TCM).[5] The TCM combines the familiar Gaussian dispersion algorithm for point sources with a simple area source algorithm suggested by Hanna and Gifford[11] to compute pollution concentrations in an urban environment. The TCM is similar in concept to the Climatological Dispersion Model (CDM)[4] in that both models are based on the same point source and plume rise equations; however, the TCM differs significantly in execution from the CDM because the point source equation is solved by interpolating in a table of precalculated coefficients and a simple equation is used to calculate concentrations due to area sources. As a result of these changes, the TCM is much faster than the CDM (roughly two orders of magnitude); but both models predict essentially the same concentrations given the same input data.

The TCM is suitable for non-reactive pollutants such as SO_2, TSP, and carbon monoxide (CO). Input to the model consists of: (1) a stability wind rose for a year or a season; (2) point source and area source parameters for two pollutants; (3) air quality monitor data for calibration (optional).

Model output from the version of the TCM used in AQMPA planning differs significantly from the published version of the model (known originally as the Fast Air Quality Model).[5] These changes are tailored to the needs of the analyst charged with control strategy development. In addition to the listing of expected concentrations and a punched card output option for isopleth mapping, the control strategy version of the TCM provides a print plot grid suitable for hand isoplething and a culpability list of the five high contributors to the concentration at each grid point.

Model Calibration

A mathematical model can, at best, only account for those physical phenomena which are described by the mathematical algorithm. Gaussian urban models such as the TCM, CDM, and Air Quality Display Model (AQDM)[14] contain algorithms that account for steady-state emissions from discrete sources defined in the inventory with well-defined meteorological conditions that change in discrete increments. The TCM and the CDM do account for some pollutant reactivity with a decay half-life term, but in practice neither model seems adequately to account for the transformation of SO_2 to sulfates. There are many important transformations which affect the concentration of pollutants in an urban environment that these urban models do not attempt to address. These transformations include meteorological conditions that vary continuously and often cannot be characterized by a single value at all altitudes of concern: reentrainment and background levels of pollution (especially important in TSP studies), pollutant reactivity (especially important in the SO_2 to sulfate conversion), and absorption by sinks (important in CO removal). The ideal solution is to modify existing models or create new models that include all important transformations of pollution in an urban environment. This is a difficult ideal to fulfill.

Reactivity, reentrainment, background, and meteorology all change drastically from urban area to urban area, and there is no simple algorithm known at this time that adequately accounts for all these important factors. There is a statistical technique, regression analysis, which can be used to relate the results of urban models to observed pollution levels. The use of regression analysis for such a purpose is generally termed model calibration. It would be much better to build a model that needs no calibration, since model calibration is easily misused. However, regression analysis is the best available method at this time to account for important transformations of the pollutant that are not adequately covered by the model algorithm.

Linear Regression

Model calibration by linear regression involves creating a scatter diagram of points (See Figure 1) that represent the observed pollutant concentration (vertical axis) versus the predicted concentration (horizontal axis). A best-fit straight line is established for the data points by the method of least squares. The equations of interest are:[2]

$$\hat{X} = a_0 + a_1 x \qquad (1)$$

$$a_1 = \left[\frac{\Sigma x_i y_i - \left(\frac{\Sigma x_i \, \Sigma y_i}{n} \right)}{\Sigma x_i^2 - \frac{(\Sigma x_i)^2}{n}} \right] \qquad (2)$$

$$a_0 = \frac{\Sigma y_i}{n} - a_1 \frac{\Sigma x_i}{n} \qquad (3)$$

where:

$\hat{X}$ = the calibrated concentration

x_i = the predicted concentration at the i^{th} point

y_i = the observed concentration at the i^{th} point

a_0 = the intercept of the line of regression

a_1 = the slope of the line of regression

n = the number of data points

A measure of how well changes in the observed data are accounted for by the model is given by the correlation coefficient:

$$r = \sqrt{\frac{\left(\Sigma x_i y_i - \frac{\Sigma x_i \Sigma y_i}{n} \right)^2}{\left[\Sigma x_i^2 - \frac{(\Sigma x_i)^2}{n} \right] \left[\Sigma y_i^2 - \frac{(\Sigma y_i)^2}{n} \right]}} \qquad (4)$$

The number of data points and the magnitude of r (ranging from 0 = no relation to 1 = perfect correlation) combine to give an estimate of the confidence we can have in the calibration of the model.[13]

where $$Z = \frac{n-3}{2} \ln \left[\frac{1+r}{1-r} \right] \qquad (5)$$

Z = the abscissa value of the normal probability curve.

TABLE 1: Confidence Level for Z Values

Z	1.96	2.575	2.81
Confidence Level	95%	99%	99.5%

Ambient Air Data

Ambient air quality data from monitors in the urban area being modeled are important elements in the calibration procedure. The monitors used should represent ambient conditions at the location being modeled. It is important that the ambient air monitor be sited properly (no wind flow obstructions), that the method used be sensitive enough to measure ambient levels, and that a large enough sample be taken to characterize the annual mean value adequately. Recommendations for monitor siting[8] and data evaluation[10] are detailed in the EPA guideline series. Because pollutant distributions at urban ambient air monitors have been found to be log-normal[12], the annual geometric mean should be used in model calibration. The problem of zero values in the computation can be avoided by assigning a value equal to one-half the minimum detectable level to measurements that fall below the minimum detectable level. However, any monitor that has recorded more than 25 percent of its values for the year below the minimum detectable level should not be used for model calibration.

Examples of Model Calibration

Figure 1 is a scatter diagram of observed and predicted values for TSP in the Dallas-Fort Worth metropolitan area for 1972. The model used is the TCM. All TSP ambient air monitors in the area were surveyed and only those monitors that were not wind flow obstructed were used to construct the calibration curve of Figure 1. Correlation and confidence level are very high for these data. The intercept of the line of regression is about 24 $\mu g/m^3$ which is a reasonable (perhaps low) number for a background TSP level. The slope of the regression line is 1.9. A possible interpretation of the slope is that TSP in the busy industrial areas is being reentrained because of the high level of human activity. This interpretation is strictly conjecture and requires support by independent tests before acceptance.

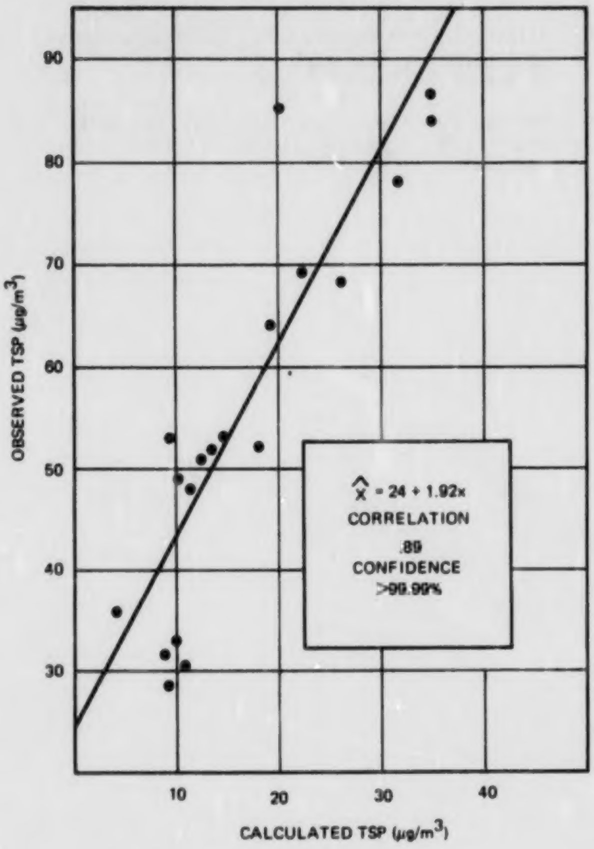

FIGURE 1. Dallas-Fort Worth, 1972, Observed versus Predicted TSP ($\mu g/m^3$)

Figure 2 is a scatter diagram of the same urban area with all monitors in the area used for calibration without regard to wind flow obstructions. The data points referring to the sites with wind flow obstructed monitors are indicated by x's, and the rest of the monitors are shown with dots. The solid line is the same regression line as Figure 1. The dashed line is a result of a least-squares fit to all the monitor data. Although there is a dramatic drop in the correlation coefficient when all sites are considered, there is very little difference in the confidence level because as r becomes smaller n increases. Since including data points whose physical relation to the model is questionable results in almost no change in the confidence level, the concept of confidence level is called into question. The critical assumption in the confidence level equation is that the n observations are independent. The independence of the observations is questionable because the means were generated from samples taken on the same days of the year (thereby experiencing the same meteorology and background) and because some of the monitors are located close enough together to be dominated by the same sources. Therefore, because of temporal and (in some cases) spatial correlation between the observations a high confidence level generated by equation (5) should be suspect. Conversely, a low confidence level generated by equation (5) can be believed. If the data will not support a Z value of at least 1.96 (95% confidence), the validity of the emissions inventory, the computer algorithm, and the air quality data should be carefully examined.

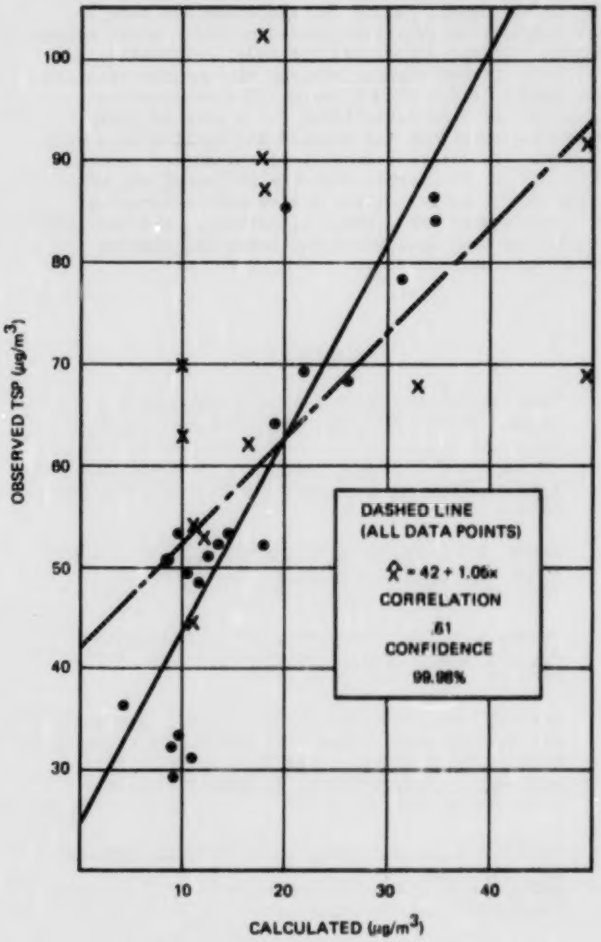

FIGURE 2. Comparison of Calibration Curves

In terms of designating an area as being in violation of the annual standard, it makes very little difference which calibration curve in Figure 2 is used. Based on the first calibration curve, all points for which the uncalibrated model predictions exceed 27 $\mu g/m^3$ would exceed the annual standard (75$\mu g/m^3$) when calibrated. Using the second calibration curve, only those points whose uncalibrated value exceed 32 $\mu g/m^3$ would be above the annual standard. This shows a degree of robustness in the calibrated model predictions with respect to the quality of ambient air monitor data and illustrates the point that the model predictions are not precision estimates. At best, the calibrated urban air pollution model indicates "ballpark" figures for projected ambient air quality.

Predicting Future Ambient Air Quality

Mathematical modeling allows the air quality planner to consider the impact of urban growth on future ambient air quality. It is necessary to project the future emissions inventory for the area being modeled.[6,7] A joint frequency distribution of meteorological elements (stability wind rose) for a period of several years should be used for climatological input to the model. The model algorithm can then be exercised using projected emissions and average meteorology. Linear regression for model calibration cannot be performed because ambient air quality data are not available for future years. The calibration equation that was established for a year of known emissions inventory and sampled air quality data must be used. Future year model projections can be accurate only to the degree that the projected emissions inventory is accurate; the future year meteorology will conform to the average climatology, and the local conditions that influenced the model calibration equation remain the same.

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A MATHEMATICAL MODEL OF DISSOLVED OXYGEN IN THE LOWER CUYAHOGA RIVER

Alan E. Ramm
Cleveland Environmental Research Group
Cleveland State University
Cleveland, Ohio

ABSTRACT

A computer model was developed to rapidly simulate dissolved oxygen content in the Cuyahoga River under varying conditions of flow and biochemical oxygen demand. The model, which has been used to simulate present and projected dissolved oxygen levels for the navigation channel of the Cuyahoga River, shows that despite the fact that industrial and municipal discharges may be completely eliminated, other factors are significant enough to cause a severe oxygen sag in the navigation channel.

BACKGROUND

Because of its recreational potential and the vast industrial complexes which span its banks depend upon it as a route for transporting raw and finished goods, the Cuyahoga River is an important river. Its importance, however, is being overshadowed by its pollution.

The current pollution problem in the Cuyahoga River is twofold:

1) The natural contour of the mouth and delta have been altered by man in an effort to make this section navigable to large vessels. These alterations have decreased the velocity of water, which has in turn decreased the river's capacity for natural aeration of water in this section; and

2) Industries and municipalities have become dependent upon the river as a receptacle for their discharged waste. This waste, which had generally been improperly treated or untreated, has created a condition of anoxia and physical degradation in certain sections of the river.

Both of the above conditions have resulted in decreased dissolved oxygen in sections of the river.

Because dissolved oxygen is vital to maintaining a homeostatic environment in stream ecosystems, one is justifiably concerned about the low dissolved oxygen content in sections of the Cuyahoga River. This concern is not only for the effect that low dissolved oxygen may have upon the plant and animal life in the river, but also for the effect that it may have upon the near shore water quality in Lake Erie.

In order to determine the effect of discharged waste upon dissolved oxygen in the river and the effect of river dissolved oxygen upon dissolved oxygen at the confluence of Lake Erie, a mathematical simulation computer model was developed. A model is advantageous for resolution of problems of this nature because parameters can be manipulated and hypothetical situations can be tested.

This model addresses itself to the problems of dissolved oxygen, and is designed specifically for use in the Cuyahoga River; however, minor alterations could make it adaptable to any stream possessing similar physical-hydraulic conditions.

The navigation channel is the dredged portion of the lower Cuyahoga River which extends from its mouth to mile point 6. Dredging maintains the navigation channel at a depth of approximately 25 feet. While lake water intrusion is generally restricted to the lower one mile of the navigation channel, the hydraulic effect of lake level fluctuations is suspected to exist throughout much of the channel. This hydraulic effect tends to increase longitudinal mixing within the channel much as tidal flux increases longitudinal mixing in estuaries. In the case of estuaries the dispersive effects of tidal fluxing are generally experienced well above that point where there is a measurable salinity change. Within the navigation channel, then, one might expect dispersion to influence water quality to varying degrees. The most significant influence is observed during periods of low flow. Because the magnitude of mixing and its significance to water quality was not previously determined, a model of the navigation channel was developed to incorporate dispersion.

METHODS

MODEL FORM

Many forms of models have been developed for estuaries in which dispersion is important and must be incorporated. Of the many forms available, the finite difference approach was selected because of its logical parallelism to the Cuyahoga River and its amenability to computerization.

Conceptually, the navigation channel was divided into twenty sections, each having a length of 0.3 miles. The choice of the number of sections was dictated by the hydrology and geometry of the channel and by the amount of computer time required to obtain a solution. Since the solution methodology requires inversion of a matrix of order N, (where N equals the number of sections in the river) as N increases the time to obtain a solution increases significantly. Each section is considered completely mixed, and hence it is assumed that no vertical or horizontal variations within a section of the river exist.

Mass balances were developed for each section with respect to DO deficit and CBOD. The balances incorporate flow from section to section and dispersion and advection between adjacent sections. Any input to or output from a given section was included in the mass balance equations for that section, as were source and sink terms for processes occurring within a section. The approach has been described in detail by Thomann, 1972 (1). The model simulates steady state conditions.

DATA REQUIREMENTS

The data required as inputs to the model may be classified under three headings: (1) coefficient determination data, (2) field data and (3) simulation run data. Coefficient determination data and field data are necessary to adapt the model's parameters to those of the Cuyahoga River system. Simulation run data is necessary to exercise the model utilizing various sets of system conditions.

The coefficients considered in the model include longitudinal dispersion, flow, benthal uptake, deoxygenation and reaeration.

Longitudinal Dispersion (D_L) within the channel was estimated from chloride distributions. Within the lower one mile, where lake intrusion is dominant, regression techniques produced estimates of longitudinal mixing coefficients on the order of 1.0-2.5 mi^2/day. It was observed that mixing effects were most intense within this region but became less intense as one proceeded upstream. Since longitudinal dispersion had never been measured upstream, the rate of decrease in magnitude of dispersion was not known. However, reasonable estimates were obtained from historical data on upstream chloride distributions. As will be noted in the following discussion, such errors as those involved in 'educated guessing' were found to be relatively unimportant to the system's general behavior.

Benthal Uptake (Sb) has never been measured within the navigation channel and consequently no data was available regarding the magnitude of this sink in the river. A decision not to design a study to measure benthal uptake was based upon current investigations being conducted at Cleveland State University. These investigations are attempting to evaluate the design of benthal respirometers of the bell jar variety.

Preliminary results of the above mentioned investigations indicate numerous problems resulting from the use of this type respirometer and tend to cast doubt upon measurements obtained from its use. Additionally, the model did not appear to be very sensitive to changes in benthal uptake (see section on Sensitivity Analysis). Since it was felt that the cost and time required to conduct such a study were not justifiable, a study of benthal uptake was not undertaken. Literature estimates of benthal uptake in rivers such as the Cuyahoga indicate a range of values from 2-10 gm/m^2/day. An estimated uptake from the channel of 5 gm/m^2/day was used.

Deoxygenation coefficients(K_1) in the lower Cuyahoga River were estimated from previous Cuyahoga River studies. Values utilized by Dalton, Dalton and Little (2) ranged from 0.2 to 0.07 liters per day (base e). These estimates were derived from an empirical equation developed by O'Connor (3) which utilized a combination of parameters, including river depth, to estimate K_1. Small variations in the value of K_1 were found to have fairly large effects upon dissolved oxygen steady-state concentrations in the navigation channel (see section on Sensitivity Analysis).

Nitrogenous Demand (Nitrification) was assumed to be negligible. Some investigators have assumed the process to be important, while others (2) considered it unlikely that nitrification occurs. O'Connor (4) suggests that nitrification is typically observed when dissolved oxygen exceeds 1-2 mg/l. This is generally true for rivers which do not receive a high concentration of various industrial wastes which inhibit bacterial growth; however, the navigation channel, because of its high industrial waste load, does not necessarily meet the conditions for this assumption. The basic arguments against nitrification are based upon the assumption that river and water quality conditions existing at critical low flow periods are not suitable for growth of nitrifying bacteria. No reliable experimental study of the nitrification process within the lower Cuyahoga exists despite the fact that loadings of ammonia are significant enough, through potential nitrification, to result in depletion of DO within the navigation channel.

Reaeration was estimated from the empirical relationship formulated by O'Connor (3).

Flow data were taken from USGS records.

RESULTS AND DISCUSSION

SENSITIVITY ANALYSES

One of the more useful applications of water quality models is to test the response of the water quality parameters under observation to changes in system parameters. By holding all but one parameter constant, it is possible to determine the relative effects of each parameter on DO. Loadings used in the sensitivity analyses were taken from Table 1, with the exception of flow which was 850 cfs in the channel.

Table 1. System Parameters For the Navigation Channel.

S	D	A	F	D	W	Sb	K_1	TEMP
1	20	3000	315	0.22	0	5	0.15	28.6
2	20	3500	315	0.22	1437	5	0.15	29.5
3	25	4200	315	0.22	0	5	0.15	30.5
4	25	4400	345	0.22	510	5	0.15	30.7
5	25	4300	345	0.22	9990	5	0.15	30.9
6	25	9000	345	0.22	0	5	0.15	31.1
7	25	4700	345	0.22	0	5	0.15	31.4
8	25	5100	345	0.22	1602	5	0.15	31.3
9	25	4900	345	0.22	0	5	0.15	31.2
10	25	5500	345	0.22	0	5	0.15	31.1
11	25	7400	345	0.22	0	5	0.15	30.9
12	25	4200	345	0.22	0	5	0.15	30.6
13	25	9000	345	0.22	0	5	0.15	30.4
14	25	6200	345	0.22	0	5	0.15	30.2
15	25	6200	345	0.22	0	5	0.15	30.2
16	25	6500	345	0.40	0	5	0.15	29.5
17	25	6500	345	0.60	0	5	0.15	28.9
18	25	4500	345	0.80	0	5	0.15	28.6
19	25	7000	345	1.00	0	5	0.15	28.3
20	25	7500	345	1.10	0	5	0.15	28.0
21	-	8200	345	1.20	-	-	-	-

S - section no.
D - depth (ft)
A - area (ft^2)
F - flow (cfs)
D - dispersion coef. (mi^2/day)
W - waste load (lbs/day)
Sb - benthal uptake (gm/m^2/day)
K_1 - deoxygenation coef. (/day)
TEMP - temperture (^oC)

Dispersion. The effect of variations in dispersion coefficients is illustrated in Figure (1A). Doubling the dispersion coefficients while holding flow and temperature constant had very little effect upon the results. This suggests that a 2- or 4- fold error in dispersion estimates would not appreciably affect the simulation output.

Benthal Uptake. Figure (1B) indicates that the maximum difference in DO which results from a 4- fold change in benthal uptake is only about 1 mg/l. Although benthal uptake has not been measured in the river, it is doubtful that it is greater than 10 gm/m^2/day. Hence an error in estimating benthal uptake by 2- to 4- fold was also not critical to the simulation of the DO sag in the channel.

Deoxygenation. Figure (1C) illustrates the results of varying the deoxygenation coefficient (K_1) in the channel. It is immediately apparent that the magnitude of the sag is quite sensitive to relatively small changes in K_1. For example, decreasing K_1 from 0.15 to 0.07 resulted in an increase of nearly 1.5 mg/l in the minimum DO. Literature values of K_1 in the Cuyahoga River ranged from 0.25 to 0.07. For critical tuning of the model a study of deoxygenation coefficients in the channel during critical low flow conditions is necessary.

Upstream Conditions. Figure (1D) illustrates the effect upon DO concentration of improving the quality of the water entering the channel. The effect of improving water quality by 1 mg/l at the head of the channel increases the minimum DO near mile point 2.0 by approximately 0.5 mg/l. To obtain water having 1 mg/l of DO at mile point 2.0 would require upstream water of better than 5 mg/l DO.

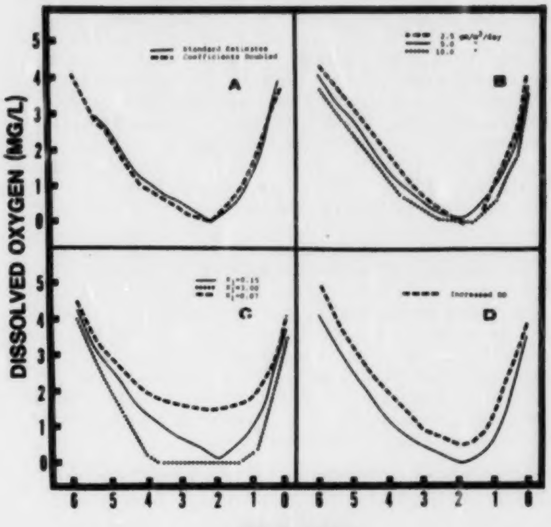

Figure 1. Sensitivity Analyses.

MODEL VERIFICATION

Because there was no data available for simultaneous DO at several locations within the channel, a sampling run was conducted in the channel on August 28, 1974 to supply this information. On this date the flow within the channel was 715 cfs. By slightly adjusting dispersion coefficients for the upper reach of the channel, it was possible to obtain a stable simulation for the river conditions on August 28, 1974. This minor adjustment of dispersion coefficients can be justified since the sensitivity analysis indicated the system to be relatively insensitive to this parameter.

The major trend in dissolved oxygen fluctuations was simulated by the model (Figure 2). From upstream to downstream the general shape of the observed data was successfully modeled. It is assumed that biological and random influences which were not incorporated in the model, resulted in the slight variations at each sample point.

Figure (2) indicates that the model is valid and, if properly utilized, can provide significant insight and understanding into DO behavior in the lower Cuyahoga River.

SIMULATION RUNS

General. A variety of simulation runs was conducted. These runs incorporated variations in waste load allocations, and input values were altered to reflect changes in waste load conditions (BOD and flow). The simulation runs were used to assess the influence of alternate waste quality control measures on the overall dissolved oxygen quality in the system.

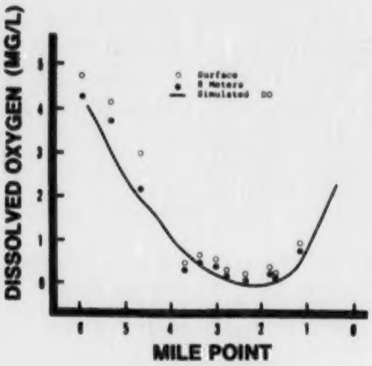

Figure 2. Verification Run.

The program was developed for input of values for cross-sectional area, flow and BOD. Cross-sectional areas at the interface of adjacent sections, where dispersion is considered, were obtained from U. S. Army Corps of Engineers' dredging maps. Where necessary, water levels were adjusted to late-summer, early-fall depths.

Flow within the navigation channel is relatively constant with respect to distance. Small increases in flow occur near the upper end of the channel due to the Ohio Canal return, and to a much lesser degree, Morgan Run and Burke Brook. Flow data utilized in the simulations conducted within the navigation channel were averages obtained from Havens and Emerson (5) and from the United States Geological Survey Water Resources Data for Ohio (6)(7). A low flow of 345 cfs and an average flow of 850 cfs were used.

Photosynthesis, a major biological source of DO, was considered to be insignificant within the navigation channel. Water is turbid and it is doubtful that any significant photosynthesis occurs except at the surface. Chlorophyll analyses of both surface and bottom water within the lower channel indicated no measurable chlorophyll.

BOD loadings were determined from Ohio EPA records. Records indicated that the majority of industries within the navigation channel which discharge significant amounts of waste are located above section 10 (m.p. 3.15). The results of simulation runs utilizing these data are presented and compared in the following.

Simulation 1. This baseline simulation illustrates the effect of present municipal and industrial discharges on water quality during low flow conditions. It was assumed that if all other water quality parameters remained constant or improved, this simulation would represent the poorest expected water quality profile for the navigation channel. System parameters for this simulation are presented in Table 1.

The results (Figure 3A) of this simulation show that discharges into Sections 2, 4 and 5 degrade water quality until the DO reaches zero in Section 5 (m.p. 4.65). More waste is discharged into Section 8 (m.p. 3.75), but its effect is not observed since DO has already reached zero. Based upon this simulation run, one would expect the river to be anoxic from Section 5 to Section 19 (m.p. .45). At Section 19 water quality improves slightly due to lake water intrusion.

The following simulation runs manipulate flow, BOD and DO to illustrate how the model can be used as a management tool. A summary of simulation runs and the variables manipulated is given in Table 2.

Table 2. Summary of Parameters used in Simulations

Simulation No	Flow (cfs)	Loading Source	Boundary Conditions Upstream BOD	Upstream DO	Downstream BOD	Downstream DO
1	345	1973-OEPA	8	3	6	6
2	850	1973-OEPA	8	3	6	6
3	345	1978-OEPA	6	3.5	6	6
4	345	50% 1973	4	4	6	6
5	850	1978-OEPA	6	5	6	6

Simulation 2. The effect of flow upon DO was tested in Simulation (3). An average flow of 850 cfs was used as the flow in the navigation channel. Figure (3B) shows that DO begins to drop slowly until zero DO is reached in Section 10 (m.p. 3.15).

When comparing Simulations (1) and (2), it is apparent that for identical conditions, river water quality during low flow is greatly reduced. This is primarily due to the low velocity and high holding time in each section during low flow. In general, it could then be assumed that water quality in the Cuyahoga River could be improved if the concentration of waste being discharged during low flow periods is reduced. This could be accomplished by temporarily storing the waste and releasing it when river flow is high or by storing water in large reservoirs and releasing it as dilution water when river flow is low.

Simulation 3. If the best practical treatment guidelines are met by 1978, it is expected that the DO in the navigation channel will improve. Projected 1978 waste load reductions were obtained from the Ohio EPA in Columbus. These values were input to illustrate the degree of improvement which could be anticipated. Results are shown in Figure (3C). Since all other conditions are identical to Run #1, the trend in DO is expected to be somewhat similar. As expected, DO drops to zero in Section 5. While water quality improves slightly as lb/day of waste load decreases, the improvement does not appear to be very significant.

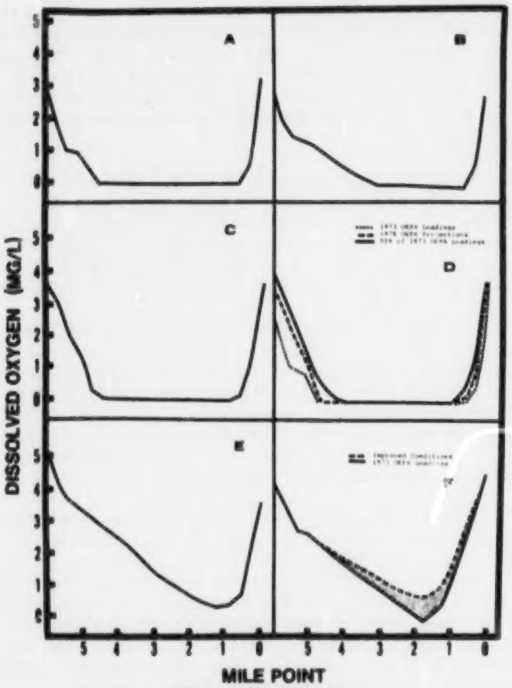

Figure 3. Simulation Runs.

Simulation 4. Simulation (4) was conducted to observe how dissolved oxygen is affected when all waste loads are decreased to 50% of 1973 values. The results of this simulation are compared in Figure (3D) with those of Simulations (1) and (3). It is apparent from the figure that water quality is only slightly improved by waste load reductions. Despite the reduced loadings, benthal uptake, upstream loadings, low rates or reaeration and long channel residence times combine to produce anoxia within much of the channel. Since the model does not reflect reduced benthal uptake rates, which might in time result from reduced loadings, these results may be somewhat pessimistic.

Simulation 5. Simulation (5) was conducted to test the combined effects of improved upstream water quality (entering DO = 5 mg/l, BOD = 6 mg/l), reduced loadings (1978 projections) and augmented flow (850 cfs.) Under these combined conditions DO dropped slowly, reaching a low of 0.35 mg/l at mile point 1.35 (Section 16) (see Figure 3E). Thus a combination of improved upstream water quality, reduced waste loading and increased flow produced a significant improvement in DO concentrations within the channel.

UTILIZING THE TRANSFER MATRIX

As the model calculates the DO deficit response for each section, the DO drop for each section is computed and listed in tabular format. The changes in DO from one section to another resulting from variations in waste load allocations can thus be directly and quickly determined from the matrix shown in Table 3. (Only half of the complete matrix is shown.)

As an example of the use of this matrix, consider the DO profile for the channel shown in Figure (3F) as "1973 channel loadings". This profile results from a flow of 900 cfs in the channel, a DO of 4.4 mg/l and a BOD of 8.0 mg/l for water entering the channel, and the waste loadings shown in Table 1.

Suppose that Republic Steel and U. S. Steel were to reduce their waste loadings to zero. This would result in a removal of approximately 10,000 lbs/days of waste from Section 5 (Republic Steel) and a removal of approximately 1,600 lbs/day from Section 8 (U. S. Steel).

Table 3 indicates the decrease in DO (Sections 1-20) resulting from waste inputs to Sections 1-10. It also can be interpreted to read the increase in DO in Sections 1-20 resulting from waste reductions in Sections 1-10. Thus a 10,000 lb/day waste removal from Section 5 would result in the increases in DO shown under 'Section 5' (Table 3). A removal of 1600 lbs/day of waste from Section 8 would produce the response obtained by taking the values from Table 3 (under 'Section 8') and multiplying each by 1600/10000 = .16).

The total response is the sum of the two responses and indicated by the line labeled 'improved conditions' in Figure (3F).

These operations allow a decision-maker to assess immediately the results of hypothetical waste load allocations without running the model. In addition, the matrix indicates that Section 16 is the most sensitive region of the channel and will receive its maximum effect (a drop in DO of 0.59 mg/l) when 10,000 lbs/day of waste is discharged into Section 5.

The transfer matrix must be recalculated (i.e., the model must be run) for different river conditions. Once the matrix is available, however, any set of waste load allocations may be applied (without rerunning the model) to observe the corresponding DO response.

Table 3. Transfer Matrix.

Section	1	2	3	4	5	6	7	8	9	10
1	-	-	-	-	-	-	-	-	-	-
2	-	-	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-	-	-
4	0.12	0.11	-	0.04	-	-	-	-	-	-
5	0.15	0.15	0.13	0.09	0.08	0.03	-	-	-	-
6	0.17	0.17	0.15	0.12	0.12	0.08	-	-	-	-
7	0.19	0.20	0.19	0.16	0.18	0.14	0.05	-	-	-
8	0.22	0.23	0.22	0.19	0.24	0.20	0.09	0.05	-	-
9	0.24	0.26	0.26	0.23	0.29	0.26	0.14	0.09	0.05	-
10	0.27	0.29	0.29	0.26	0.35	0.32	0.18	0.14	0.10	0.07
11	0.28	0.31	0.32	0.29	0.39	0.37	0.22	0.18	0.14	0.12
12	0.31	0.34	0.35	0.32	0.45	0.43	0.26	0.23	0.19	0.19
13	0.32	0.36	0.37	0.35	0.49	0.46	0.29	0.26	0.23	0.23
14	0.34	0.38	0.40	0.38	0.53	0.51	0.32	0.30	0.27	0.28
15	0.36	0.40	0.42	0.40	0.57	0.56	0.36	0.34	0.31	0.34
16	0.36	0.41	0.43	0.41	0.59	0.58	0.58	0.36	0.33	0.37
17	0.34	0.39	0.41	0.40	0.57	0.56	0.37	0.35	0.33	0.37
18	0.26	0.29	0.31	0.30	0.44	0.43	0.28	0.27	0.26	0.29
19	0.18	0.20	0.22	0.21	0.30	0.30	0.20	0.19	0.18	0.20
20	-	0.10	0.11	0.10	0.15	0.15	0.10	0.09	0.09	0.10

SUMMARY

By utilizing the model it is possible to answer several types of questions which must be addressed by management:

Question 1:	How can the model determine the upstream water quality required to achieve the water quality standards set for the Cuyahoga River's navigation channel?
Answer 1:	In order to maintain the standards set for the river, water quality in sections 14-16 must be controlled. Therefore, upstream flow, BOD, DO and waste inputs must be manipulated until an acceptable DO is obtained in Sections 14-17. Simulations 1-5 demonstrate the expected changes which would occur when manipulating each of these parameters. Additional manipulations require only changing the input data.
Question 2:	How can the model be utilized to determine the best physical system for achieving that water quality?
Answer 2:	Once the desired DO level is obtained in Sections 14-16, one must then determine the most economic or most efficient means for effecting the required changes. For example, if flow is doubled and BOD is decreased by half, then one must decide how to double the flow and decrease the BOD. Such alternatives as storing dilution water to augment flow, eliminating all discharges, etc., must be approached from an economical point of view; however, the response to using combinations of the different alternatives can be observed from the model.
Question 3:	How can the model assist in determining the optimal system for administering and managing water quality?
Answer 3:	The Transfer Matrix (Table 12) provides an excellent tool for determining the optimal locations for outfalls and the optimal waste load inputs because this matrix points out the sections which can least tolerate and most tolerate a waste load.

Through an understanding of the complex physical, chemical and biological events occurring simultaneously within the system, the model has demonstrated its ability to simulate the dissolved oxygen profile in the river. The oxygen profiles resulting from use of the model, when compared with field measurements, provided a reasonable fit. The model, therefore, allows a water planner to assess the impact of alternate water quality control measures on the river system by varying the treatment levels at each discharge point and the water quality conditions in Lake Erie at its mouth. By increasing flow, while holding discharge constant, the model can also estimate the volume of dilution water required to meet dissolved oxygen standards in the river.

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A WATER RESIDUALS INVENTORY FOR NATIONAL POLICY ANALYSIS

Edward H. Pechan*
Consultant
National Academy of Sciences
Washington, D.C.

Ralph A. Luken**
Consultant
National Academy of Sciences
Washington, D.C.

ABSTRACT

A computer based water residuals generation and discharge inventory was developed to assist in the evaluation of regional and national implications of the uniform effluent requirements of the Federal Water Pollution Control Act Amendments of 1972 (PL 92-500) and in the evaluation of alternative residuals control policies.

The completed system, termed the National Residuals Discharge Inventory (NRDI), has been used in a number of applications including the investigation of costs, residuals discharge, and residuals dilution effects of three alternative policies to national uniform effluent standards.

BACKGROUND

The Federal Water Pollution Control Act Amendments of 1972 (hereafter referred to as P.L. 92-500 or the 1972 Act) marked a decisive shift in the nation's approach to restoring and maintaining the physical, chemical, and biological integrity of its waters. That shift is best reflected in the major change in enforcement mechanisms. Under prior legislation, ambient water quality standards were set as the control mechanism. The use of the waters for such activities as drinking, recreation, and manufacturing determined the kinds and amounts of residuals to be discharged, the degree of residual abatement required, and the rapidity with which dischargers were to install the necessary abatement technology. Under the 1972 Act, effluent limitations were set as the control mechanism. The existence and availability of water pollution control technology determined the kinds and amounts of residuals to be discharged, and legislatively mandated compliance dates determined the rapidity with which dischargers must install the necessary abatement technology.

The overwhelming Congressional support for the 1972 Law resulted from disillusionment with the lack of progress under more than two decades of Federal legislation. Contributing problems to the failure of previous efforts were the tardiness of the States in setting water quality standards, the complex procedures which delayed enforcement actions against polluters, and the failure to fully implement the Federal construction grant program for municipal sewage treatment facilities.

The 1972 Act attempted to respond to these limitations with three essential elements; uniformity, finality, and enforceability. Uniformity is mandated by the requirement that each residual discharger within a category or class of industrial sources and all municipal sources must meet stipulated effluent limitations regardless of geographic location. Categories or classes of industrial sources will be required to meet unique, nationally uniform, effluent limitations based on "best practicable control technology currently available" (BPT) by 1977, and to meet even more stringent nationally uniform effluent limitations based on "best available technology economically achievable" (BAT) by 1983. All municipal sources (publicly owned treatment works) will be required to meet effluent limitations based on secondary treatment (ST) by 1977 and based on "best practicable wastewater treatment technology" (BPWTT) by 1983.

Finality is mandated by the requirement to meet more stringent effluent limitations by point sources (municipal and industrial activities) at specific dates in the future. While prior legislation did not set specific dates for meeting water quality goals, the 1972 Act requires dischargers to meet one set of effluent limitations in 1977, a more stringent set of effluent limitations in 1983, and looks toward achieving a final goal of zero discharge of pollutants into navigable waters by 1985. In addition, an interim goal of achieving waters fit for fishing and swimming by 1983 is established. The concept of finality is intended to remove the uncertainty on the part of industrial and municipal dischargers about the nation's (or at least Congress') commitment to maintaining and restoring the quality of the nation's waters.

Enforceability is assured through the provisions of the permit program and the new enforcement authorities given to the EPA. The 1972 Act is based on the assumption that violations of permit conditions would be easier to determine than violations of water quality standards, assuming the ability to design an adequate compliance monitoring program and to inspect the operations of residual dischargers. EPA not only has the authority, but is required to issue an abatement order whenever there is a violation of the conditions of a permit and a state fails to move against the violator in a timely fashion. Furthermore, a citizen may bring suit against EPA if it fails to issue a necessary order.

Although the 1972 Act received Congressional support in its final form sufficient to override a Presidential veto, there were many compromises in the development of the final version as it moved through the procedures of the Congress. Thus, while the three major innovative provisions of the Senate version survived in the legislation agreed to by the Conference Committee, a provision was inserted to establish a National Study Commission to "make a full and complete investigation and study of all of the technological aspects of achieving, and all aspects of the total economic, social and environmental effects of achieving or not achieving the effluent limitations and goals set forth for 1983 ..." (P.L. 92-500) looking toward recommendations not later than October 18, 1975 as to any needed "... mid-course corrections that may be necessary ..." (H.R. 92-1465).

In implementing its study program, using the efforts of almost 100 contractors, the National Commission on Water Quality (NCWQ) appeared to accept the uniformity provisions of the Act and defined its contract studies to concentrate primarily on the finality provisions and secondarily on the enforceability provisions. None of the studies questioned the benefits or costs of requiring uniform treatment of similar classes of residual discharges regardless of geographic location.

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* Mr. Pechan is currently with the U.S. Energy Research and Development Administration in Washington, D.C.

** Dr. Luken is currently with the United Nations in Bangkok, Thailand.

Early in the course of its study program, the NCWQ contracted with the National Academy of Sciences/ National Academy of Engineering/National Research Council under the provisions of Section 315 for assistance in particular areas of concern.

In order to provide the assistance needed, the Environmental Studies Board of the National Research Council created the Study Committee on Water Quality Policy (CWQP). In connection with its accomplishments of the tasks assigned by NCWQ, CWQP determined that an independent assessment of residual reduction technologies was essential to provide perspective on its assignment. In the absence of a breakdown by NCWQ of national totals by geographic regions, primarily due to inability of the Strategic Environmental Assessment System (SEAS) to accurately compute and display (by region) data from the contractor studies, CWQP engaged consultants and directed them to devise a system which could provide it with a basis for an independent analysis of the effects of achieving or not achieving the goals of the Act.

NATIONAL RESIDUALS DISCHARGE INVENTORY

To provide a basis for handling the immense amount of data available from the NCWQ contractor's reports, from the U.S. Environmental Protection Agency (EPA) and from other available sources, the consultants devised a system for computerized analysis called the National Residuals Discharge Inventory (NRDI).

The NRDI analysis was to provide a basis for the CWQP's comments on the NCWQ's contractor and staff draft reports. It was also hoped that the analysis would be of value to the NCWQ as it moved toward preparation of its own final report.

To carry out this assignment, the CWQP consultants were requested to:

- document the distribution of residual generation and discharges by region;
- document the distribution of residual generation by activity;
- describe the relative importance of activity categories by region;
- document the distribution of residual reduction technology cost by region;
- indicate the sensitivity of estimates of residuals generation, discharge, and reduction technology costs to various assumptions;
- evaluate the quality of basic data on residual generation, discharge, and technology used by NCWQ contractors and describe other possible data sources.

NRDI is a quantitative assessment of residual generation and discharges and of residual reduction technology costs in each of the 3,111 counties or county approximations in the contiguous U.S. Data for industrial, municipal, urban runoff, and non-irrigated agriculture sources are available for each county. However, the data are not displayed at the county level, but rather are aggregated for purposes of analysis by the Water Resources Council's 99 aggregated sub-areas (ASAs), the 18 Water Resource Regions (WRRs) and by the nation. The ASAs and WRRs are often generically referred to in this report as river basins.

The purposes of NRDI are: (a) to provide a comprehensive measure of biological oxygen demand (BOD), total suspended solids (TSS), nitrogen (N), and phosphorus (P) residual generation and discharge aggregated for the nation and for each of the 18 WRRs and 99 ASAs, (b) to indicate the relative importance of various activities as sources of residuals after the effluent limitations for 1977 and 1983 are met; (c) to provide a comprehensive measure of the costs of residual reduction technologies required to meet the 1977 and 1983 technological objectives of the 1972 Law aggregated for the nation, the 18 WRRs, and the 99 ASAs, and (d) to estimate the cost savings to the nation of pursuing alternative policies. The NRDI analyses include point sources, which are defined as discharges from municipal and industrial activities, and areal sources, which are defined as urban runoff and drainage from non-irrigated agricultural activities.

Thus, NRDI is a conceptually simple but systematic computational procedure for evaluating various aspects of the 1972 Law. The inventory has the capacity to predict potential reductions in residuals discharged into the ambient environment and the associated costs of the application of uniform residual reduction technologies stipulated by EPA for municipal and industrial residual generators. It can compare the resulting reductions in discharges from these sources with those from other sources, primarily urban storm water runoff and non-irrigated agriculture, by river basins. More importantly, NRDI allows for an evaluation of policy alternatives to the uniform application of residual reduction technologies to legislatively defined (P.L. 92-500) point sources. These policies reflect alternatives where in a given river basin, achievement of the 1983 effluent limitations would not make a significant improvement in total residual reductions and ambient water quality, and where a given level of residual reduction could be achieved at a lower cost without the uniform application of residual reduction technology to point sources.

NRDI consists of (a) inventories of production and consumption activities which generate and discharge residuals, (b) a system for analyzing the effects of increased industrial production and population growth, (c) an index of potential water quality changes, and (d) residual discharge reduction policies which include the BPT/ST and BAT/BPWTT technology goals in the Act.

ACTIVITY INVENTORIES

The purposes of the activity inventories are twofold. First, the inventories relate process/production data to residual generation coefficients for calculation of residual generation for a particular activity. Second, the inventories assign an appropriate residual reduction technology, as specified under the policy alternatives, thereby enabling the computation of abatement costs and of residuals discharged into the ambient environment. The specificity of the individual activity inventories for the above process depends upon the importance of each sector as a residual generator and upon the availability of data.

The data input files for activity inventories contain information on identifiable point and areal source residual generating activities. The point and areal activities combined cover most major waterborne residual generating activities. Information included about these activities, where appropriate and available, are location of activity, measures of production (physical output, employees, land area, or population) type of production process, and current residual reduction technologies being used.

There are several activity inventories for the municipal, industrial, and areal categories. The municipal category includes a sewage treatment plant inventory based on the 1974 EPA Needs Survey[1]. The industrial category includes an in depth industry inventory for the significant process water users and a general industry inventory for the vast majority of other residual generating industries (Table 1).

TABLE 1 - NRDI INDUSTRY STUDY CATEGORIES

INDUSTRIES STUDIED IN DEPTH

Pulp and Paper
Petroleum Refining
Textiles
Iron & Steel

Plastics & Synthetics
Organic Chemicals
Inorganic Chemicals
Steam Electric

INDUSTRIES STUDIED IN GENERAL

Ore Mining
Coal Mining
Petroleum & Gas
Mineral Mining
Meat Processing
Dairy Products
Grain Mills
Cane Sugar
Beet Sugar
Seafood
Builders Paper
Fertilizer

Paving & Roofing
Rubber
Leather
Glass
Cement
Pottery
Asbestos
Ferroalloys
Non-ferrous Metals
Electroplating
Fruits & Vegetables
Other Organic Chemicals

Industrial plant data for the in-depth industries was developed from numerous sources as described in the NRDI report[2]. Plant data for the general industries was obtained from Census data[3]. Residuals generation and water use information was obtained from both EPA Development Documents and Census data[4].

Residual generation coefficients for industries studied in depth are specified for each production process within an activity category. For the industries studied in general, total residual generation for a four-digit SIC category is used. The coefficients are given as weights of residuals per production output unit (for example, pounds of organic residuals generated per ton of pulp or per barrel of crude oil processed). The residuals included are BOD, TSS, and wastewater flow.

The input file also specifies the various residual reduction technologies available for each of the activities. Information specified for each technology or unit process includes costs and residual reduction rates or removal efficiencies.

Areal sources include urban runoff and non-irrigated agriculture, both analyzed by county. Information for the urban runoff was obtained from the Needs Survey, Census data[5], and an NCWQ contractor report[6]. Counties were included which were (1) part of an SMSA and (2) had an average resident population density of .6 persons per acre or more.

Non-irrigated agriculture activities were defined on a county-by county basis by acres under cultivation, soil types, etc. Residuals were computed by successive application of the uniform soil loss equation, sediment delivery ratios, and residuals carried by sediment. The single control policy was developed by simulating the application of soil conservation measures as outlined in the 1967 Conservation Needs Inventory.

Estimated residual delivery and costs of control were obtained from the NCWQ contractor[7]. The sediment delivery ratios were back-computed and residual loadings were adjusted to correspond with Iowa State Sediment delivery ratios[8].

The costs of residual reduction technologies are computed for the capital or initial investment cost.

GROWTH ANALYSIS

The purpose of the growth analysis is to project future levels of residual generation and discharge. The projected growth for industry is based on increases in physical output growth while that for municipalities is based on population growth rates. Growth is not projected for urban runoff or non-irrigated agriculture activities. While the growth analysis design permitted either national or ASA averages for industrial and municipal sectors, as a first approximation, only the former have been used to date.

The growth assumption does not generally influence the results of the analysis presented here which is based only on 1973 data.

Inputs into the growth analysis are projected industrial production and population increases. The projected growth for industry is available either from the Wharton Economic Forecasting Analysis used by NCWQ[9] or the U.S. Department of Commerce, OBERS Series E[10]. The projected growth for municipalities is based on U.S. Department of Commerce, Census Series E population growth rates.

RESIDUALS DILUTION RANKING INDEX

The purpose of the water quality indexing procedure is to convert the information on residuals discharged into an approximate measure of water quality. The procedure is essentially a mechanism for ranking the basins according to relative average water quality, i.e., "average" conditions are determined for each basin and the basins ranked accordingly. Such a ranking may then be used to identify those ASAs which are relatively well off or have problems under current conditions and which may be significantly affected by different water quality management policies. Since the "average" conditions do not reflect a real situation at any given location or time, they cannot be used to attempt to pinpoint specific water quality problems in a sub-basin or stream segment.

At this time, the only water quality related data unique to each river basin are approximations of low and average flow conditions and number of stream miles.

OUTCOME SUMMARIES

The outputs resulting from each policy alternative are:

- residual generation;
- residual discharge;
- abatement costs;
- residuals dilution index.

These outputs must be taken together to evaluate a given policy, because no one output is by itself an adequate evaluation measure. However, even the combination is no substitute for basin specific evaluation. At that level of detail, data are available for assessing actual changes in physical, chemical and biological parameters and for measuring the damages which are sustained directly by human beings or indirectly by plants and animals of value to man.

ALTERNATIVE POLICIES

A variety of alternative policies can be selected for solution in the NRDI. These policies include both uniform and non-uniform abatement policies and can simulate controls on areal as well as point sources.

In using the model, a target year for analysis is selected. Standard years are 1973 (base case), 1977, and 1983.

The model has been exercised with a variety of abatement policies. Due to the simplicity of the model, it is relatively easy to add new policies. The basic policies used to date are discussed below:

a. No control - This policy estimates risiduals discharge if no control technology is used.

b. 1973 controls - This policy estimates discharge and costs based on control technology in place in 1973.

c. BPT/ST - This policy estimates effects of the 1977 standards of the Act: Best Practicable Treatment for industry and Secondary Treatment for municipalities.

d. BAT/BPWTT - This policy estimates effects of the 1983 standards for industry and secondary treatment for municipalities supplemented with tertiary facilities when requested in the Needs Survey.

e. BAT/BPWTT$^+$- This policy is identical to (d) for industrial sources but includes filtration for all municipalities not requesting treatment more stringent than secondary in the Needs Survey.

f. Non-irrigated agricultural control - Costs and residual implications of implementing practices outlined in the 1967 Conservation Needs Inventory are included.

g. Urban storm control - Costs and residual implications of one of five urban storm control strategies (combined, separate storm, and unsewered) is simulated.

h. Ocean discharges - Effects of discharge and costs for ocean counties are excluded. This function is used to simulate lower levels of treatment for ocean discharges based on using a specified set of counties.

i. New Source Performance Standards - In this policy, residual discharges and costs for industrial growth are based on new source performance standards (approximated by BAT).

j. Limited technology - Simulation of stringent effluent limitation policies can be limited to ASAs with relatively bad water quality.

k. Cost effective strategy - This policy used data on cost per quantity of residuals removed to identify cost-effective solutions in each ASA.

Combinations of these policy components can be combinned in a single run if desired.

RESULTS

Illustrative results and conclusions are presented in this paper. The results presented show the costs of uniform application of BAT/BPWTT, as well as three policy alternatives.

Table 2 presents summary results of the policies. The results of the illustrative alternatives to the uniform application of BAT/BPWTT are discussed below.

TABLE 2 - COMPARISONS OF ALTERNATIVE POLICIES

	BOD Removed	Total Capital
Technology	10^9 lbs/yr	10^9 1975 $
Uniform BPT/ST	7.4	38.5
Uniform BAT/BPWTT	8.8	55.6
Alternative I	8.0	43.2
Alternative II		
Cost-eff. BPT/ST	7.4	23.0
Cost-eff. BAT/BPWTT	8.8	37.0
Alternative III		
EPA counties	8.7	55.2
Potential counties	8.6	52.9

Alternative I: Limit BAT/BPWTT Technology Investment to Areas with Relatively Poor Water Quality

One alternative is to require that the BAT/BPWTT technology objectives be met only in those areas (ASAs) which have relatively severe water quality problems. This alternative limits the application of BAT/BPWTT technologies to ASAs which have a BOD dilution index equal to or greater than 3.0 mg/l. The result of this alternative is that if uniform water quality is a policy objective, it can be obtained for only $5.7 billion more than BPT/ST, a reduction of $12.5 billion from the costs of uniform BAT/BPWTT. This is achieved by applying the more stringent effluent limitation to 21 instead of all 99 ASAs. The results suggest that in the remaining areas (78 ASAs) BAT/BPWTT may not really be necessary because they generally may have met water quality standards after BPT/ST. Areas (ASAs) with no additional cost, in this case, would be located in the New England, Tennessee, Upper Mississippi, Lower Mississippi, Upper Colorado, and Pacific Northwest WRRs. This alternative illustrates that if the ultimate goal of the law is to restore the nation's water quality, then it can be achieved at lesser cost

Alternative II: Invest Only in Cost Effective Options

The second alternative is to require only those sources which have the least cost to invest in more stringent technology in order to achieve the residual reduction accomplished by uniform BAT/BPWTT. This alternative is based on considering all major sources of residuals, including urban runoff and non-irrigated agriculture, and applying both BPT/ST and BAT/BPWTT non-uniformly in order to achieve a given level of residual reduction for the least costs.

The results showed that a 33 percent reduciton in total BPT/ST and BAT/BPWTT costs, 41 percent for BPT/ST and 12 percent for BAT/BPWTT, can be obtained, and the same quantities of residuals removed, by substituting a nonuniform cost effective policy approach for uniformity. The five regions (WRRs) that benefit the most from a cost effective approach include the Upper Mississippi, Lower Mississippi, Missouri, Rio Grande and Arkansas-White-Red Water Resource Regions.

This alternative suggests that if the quantities of residuals removed after uniform BPT/ST and BAT/BPWTT are policy objectives, then they can be achieved at lesser costs.

Alternative III: Do Not Invest in BAT Technology in Areas with Potential for Ocean Discharge

The last alternative is to not require point source dischargers in all counties which have the potential for ocean discharge to meet the BAT/BTWPP technology objectives. This alternative is based on computing a lower bound, which excluded point dischargers in selected counties in only three regions with generally recognized assimilative capacity, and an upper bound which excluded point source dischargers in selected counties in regions with potential tidal dilution capacity. The lower bound resulted in a national cost saving of $0.4 billion or only two percent of the NRDI estimated BAT/BPWTT costs while the upper bound considered 172 counties and resulted in a national cost savings of $2.7 billion. Savings included fifteen percent of the uniform BAT/BPWTT costs for the California region and twenty-eight percent for the Pacific Northwest. This alternative illustrates that if the nation is willing to use the natural assimilative capacity of the oceans, a few regions would achieve a significant reduction in BAT/BPWTT costs.

In summary, we examined three illustrative alternatives to the uniform application of the technology standards. These alternatives could conceivably yield savings of between 2 percent and 70 percent of the costs of meeting uniform standards without a significant deterioration of either the residual reductions or the water quality gains achieved using the uniform policy. Since these alternatives are not mutually exclusive, all or some of them could be adapted simultaneously and result in a significant percent reduction of the costs of uniform standards. Of course, more detailed analysis would be needed including consideration of institutional issues and methods of implementation before a new approach is adopted.

CONCLUSIONS

Analysis done to date with the NRDI has shown it to be a powerful tool which can be used to examine the effects of various abatement policies at a regional level. The model is unique in its capability of simultaneously estimating costs, residuals discharge, and residuals dilution effects of alternative policies.

Major limitations of the system include its omission of some important sources i.e. silviculture, construction, its limited coverage of residuals, and our limited faith in the "water quality" estimates.

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A MULTI-PARAMETER ESTUARY MODEL*

Paul A. Johanson
Tetra Tech, Inc.
Lafayette, California

Marc W. Lorenzen
Tetra Tech, Inc.
Lafayette, California

William W. Waddel
Washington Public Power
Supply System
Richland, Washington

ABSTRACT

To obtain information needed in the development of a water quality plan for Grays Harbor, in Washington State, the mathematical water quality model EXPLORE was modified for application to the harbor and the lower Chehalis River. This report describes the model selection criteria and the procedures used in applying the model to a tidally influenced estuary and river.

Results of the study show that model calculations and observed data correlate well, confirming that the model is a valuable tool for evaluating the effects of various waste discharge schemes on the quality of a water body and thus for helping to select a plan for managing water resources. The study also indicates that further information about rates of benthic oxygen demand and the oxygen content of incoming seawater would improve the accuracy of the model calculations.

INTRODUCTION

The need for high quality water to maintain natural productivity and the need to assimilate waste materials often conflict in estuarine areas (1). Careful management of water resources is essential in these areas, and one tool which can be of immense help to the engineer/planner is mathematical simulation. Through the use of computer models it is possible to describe quantitatively the behavior and interactions of various water quality parameters and thereby predict the effects of various management schemes.

This report describes the modification of a mathematical model for application to a particular estuary system. Water quality problems and conflicting water uses in the estuary have indicated the need for more careful resource management, and water quality modeling can be of obvious benefit.

PURPOSE AND CONCLUSIONS OF THE STUDY

Application of the Battelle-Northwest EXPLORE water quality model to Grays Harbor and the lower Chehalis River in Washington State was the major task of a recently completed program. The purpose of the study was to provide specific information needed to develop a water quality management plan for Grays Harbor County. It was felt that mathematical modeling techniques would provide the best method of evaluating the effects of various waste discharge schemes on the water quality of Grays Harbor.

This report reviews the characteristics of a water quality model needed for this task and discusses calibration and use of the model. Results are in reasonable agreement with observed data and show the utility of the model as a water management tool.

Results of this study indicate that further information is needed about rates of benthic oxygen demand and the oxygen content of incoming seawater, and field measurements of these parameters are suggested.

CAPABILITIES REQUIRED OF THE MODEL

Water quality modeling in an estuarine system requires the determination of water flows, depths, and velocities in order to properly transport the quality parameters through the system. Thus, hydrodynamic calculations are prerequisite to any quality calculations. Once the physical transport of water has been determined, biological and chemical reactions can be superimposed to calculate water quality at any location and time.

The primary quality parameter of concern in Grays Harbor is dissolved oxygen (DO). Low oxygen concentrations have been observed in the estuary during periods of low flow. DO is predominantly a function of biochemical oxygen demand (BOD) discharged to the system, benthic oxygen demand, surface reaeration, and algal growth and decay. BOD and benthic oxygen demand depend on wastes discharged to the system. Surface reaeration depends on water and wind velocities as well as oxygen deficiencies. Algal growth and decay rates depend on nutrient concentrations, light penetration, temperature and possibly toxic substances discharged to the system.

The EXPLORE model is derived from a hydrodynamic code developed by Water Resources Engineers (WRE) (2). Whereas standard approaches to the solution of unsteady flow equations generally represent varying methods of making the equations numerically discrete, the approach adopted by WRE involves a discretization of the physical system being modeled. The region is subdivided into a number of nodes with channels connecting adjacent nodes. The continuity equation is solved at junctions or node points while the momentum equation is solved along connecting channels. This approach has been applied successfully to the simulation of estuarine networks of the Sacramento-San Joaquin Delta by WRE and to the Columbia River by the Environmental Protection Agency. The general purpose computer program originally written by WRE was later modified, updated and refined by the Federal Water Pollution Control Administration and is reported by Callaway, Byram and Ditsworth (3) and Feigner and Harris (4). More generalized versions of the code have been incorporated into the Storm Water Management Model (5) and the Battelle-Northwest EXPLORE Program (6).

MODEL SELECTION

The Battelle-Northwest EXPLORE hydraulic code was chosen for use in the Grays Harbor-Chehalis River estuary for three reasons: it has been successfully tested and used for a number of different simulations; it can be effectively applied to an estuary with the physiographic features of Grays Harbor; and a number of water quality programs have been written for use with this code.

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*This work was completed under partial support of Contract 68-01-1807 of the Environmental Protection Agency in Oct. 1974, while the participants were employed at Battelle Northwest Laboratories, Richland, WA. The assistance of Charles R. Cole of BNW is gratefully acknowledged.

The three most widely used of these water quality models are discussed in references 4, 5 and 6. The EXPLORE quality code was selected because it is the most comprehensive and versatile of the three programs and because it was written for maximum compatibility with the EXPLORE hydraulic code.

The water quality models used were developed by Battelle-Northwest for the Environmental Protection Agency to serve as a management tool in the study of water resources and pollution abatement programs. The models afford an overall perspective of the synergistic effects of various proposed plans.

Not all of the water quality models were used in the present modeling effort due to a lack of data for calibration, but other constituents can be studied when more data become available.

A detailed description of the procedure for using the EXPLORE code has been given elsewhere (7). Briefly: the study area is divided into nodes and channels. Surface area and depth are determined for each node, while length and width are measured for each channel. The process of dividing the area into nodes requires experience, three considerations being paramount: areas of great concern (such as waste discharges, municipal areas, or regions characterized by low water quality) or requiring great detail will generally require a large number of nodes; channels must be longer than a limit which is determined by the timestep used; and more detailed systems involve greater expense in data preparation and computational time.

Tributary stream flows are added as either time-varying or constant values, upstream control points and tidally controlled nodes are established and the tidal regime is chosen. The hydraulic code then calculates flows and velocities for each channel and water surface elevations and volumes for each node as functions of time. The code is allowed to run for a number of tidal cycles until steady-state conditions are established. Although the code can handle transient conditions, only average diurnal variations are considered for specific conditions such as low flow periods. This is so because the effect on the predicted water quality of transient conditions caused by variations in tidal cycles and river flows is usually small for the short period of time for which the simulation is performed. By averaging the variations the computational time is reduced, which significantly reduces costs without compromising the usefulness of the results.

Utilizing the output from the hydraulic code in conjunction with the quality of the waste sources and initial conditions of each water quality parameter, the quality code calculates the concentrations of all the parameters as functions of time and location. The values of constants which are not known are set so that the computer output simulates field observations. Once the model is calibrated, the locations and magnitudes of waste sources can be varied to evaluate the effects of different management schemes.

CALIBRATION AND VERIFICATION

Hydrodynamic Model

In order to calibrate the hydrodynamic portion of the model, stream flow and tidal data were needed. August 15-20, 1971, was chosen for calibration because quality data for this period were available. High and low water predictions from Department of Commerce Tide Tables were chosen to describe the time-stage curve, and river flow data for the same period were taken from Water Resources Data for Washington.

Water Quality Model

Because sufficient data were not available with regard to chemical concentrations, algal nutrients, and photosynthetic processes in Grays Harbor, only BOD, benthic oxygen demand, and surface reaeration were considered in the model calculations. Information about sources of major BOD discharge were obtained from the State Department of Ecology.

The dissolved oxygen concentrations measured in the Harbor for 1970, 1971 and 1972 were taken from Interim Reports and from raw data supplied by the Department of Ecology.

Initial calculations showed that waste discharges alone would not account for the low observed DO. It became apparent that a benthic oxygen demand would have to be assumed in areas where waste discharges occurred, a reasonable assumption since organic matter would be expected to settle to the bottom in such areas and create an oxygen demand. The values used were chosen to correctly simulate the observed oxygen concentrations in the estuary for 1971 and were not changed for the 1970 and 1972 verification periods other than to examine the effect of eliminating benthic demand. There is probably some benthic oxygen demand throughout the estuary, but assumption of values was considered to be warranted only in the areas where oxygen data were available for calibration.

In the process of analyzing the oxygen field data it was observed that although less BOD was discharged to the North Channel during 1970 than in 1971, the measured oxygen concentrations were lower in 1970 than in 1971. The most logical explanation for this observation is that incoming ocean water must have been lower in dissolved oxygen in 1970 than in 1971. For this reason the 1970 incoming ocean water oxygen concentration was fixed at 6.0 mg/l. In 1971 and 1972 the incoming oxygen concentration was set at 7.0 mg/l.

Figures 1, 2, and 3 show computer predictions (curves) and data for five consecutive days (points) for 1970, 1971, and 1972. DO is plotted against Department of Ecology station numbers (lower axis) and node numbers (upper axis)

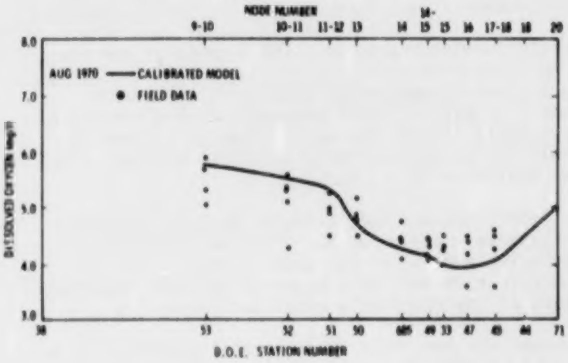

Figure 1.

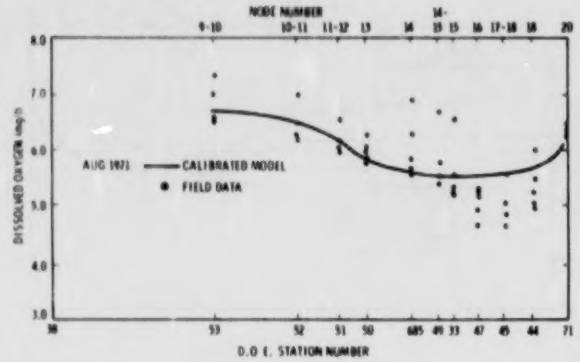

Figure 2.

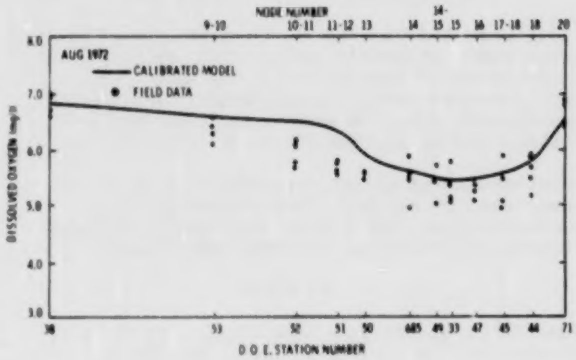

Figure 3.

SENSITIVITY ANALYSIS

In each of the sensitivity studies lowest DO was found to occur in the same general area, so the figures show only this region.

The importance of benthic oxygen demand in 1970 is illustrated in Figure 4. The model predictions, with the elimination of benthic oxygen demand, are shown with the calibrated model predictions for 1970. It is readily apparent that the benthic demand used in the model contributes significantly to the predicted oxygen sag. Figure 5 shows the predicted oxygen concentrations with no benthic demand and a reduced reaeration coefficient. It is apparent that some other combination of lower benthic BOD and reaeration coefficients could have simulated the data. However, it was felt that the values used were the most appropriate.

Figure 6 illustrates the effect of removing the benthic oxygen demand for the 1972 flow conditions. With no benthic demand, the predicted oxygen concentrations are significantly higher than the calibrated model had predicted. A comparison of Figures 4 and 6 reveals that the benthic oxygen demand was more important in producing the oxygen sag during the 1972 period than during 1970. This result is consistent with the fact that industrial discharges were lower in 1972 than in 1970. As the discharged BOD is decreased, the contribution of benthic demand becomes more important in the total oxygen balance

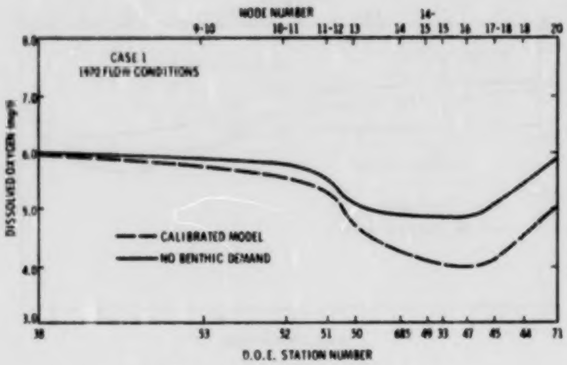

Figure 4.

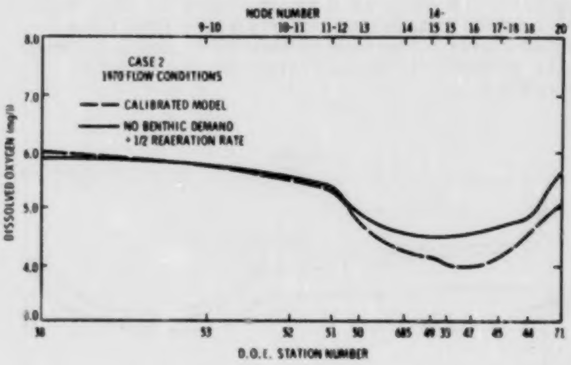

Figure 5.

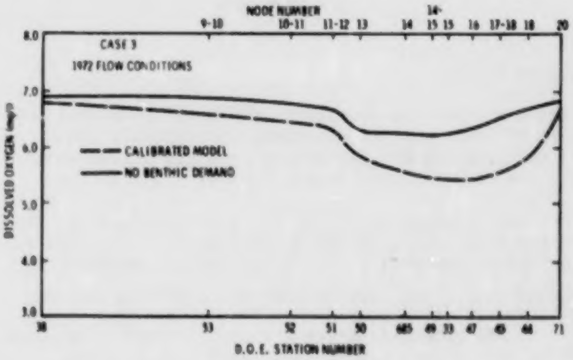

Figure 6.

The effect of eliminating industrial discharges of BOD is shown in Figure 7. The model was run with ocean DO set at 6.0 and 7.0 mg/l. Minimum DO occurs in approximately the same point for each of these cases and ranges from 5.8 mg/l to 6.2 mg/l. Benthic demand would be expected to gradually decrease under these conditions but the rate of change is not known.

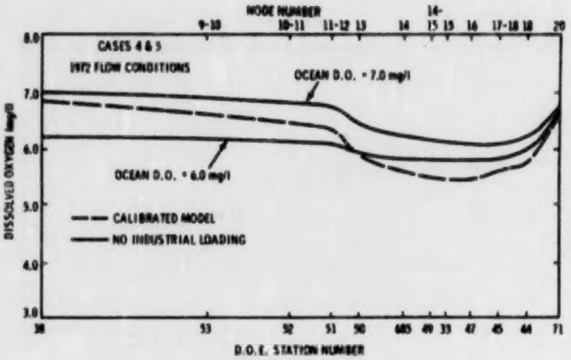

Figure 7.

The effects of the proposed Department of Ecology discharge limits were simulated with ocean DO of 6.0 mg/l and 7.0 mg/l, as shown in Figure 8. The observed 1972 conditions do not differ greatly from the proposed limits. The results show that proposed limits will probably not be sufficient to meet quality standards.

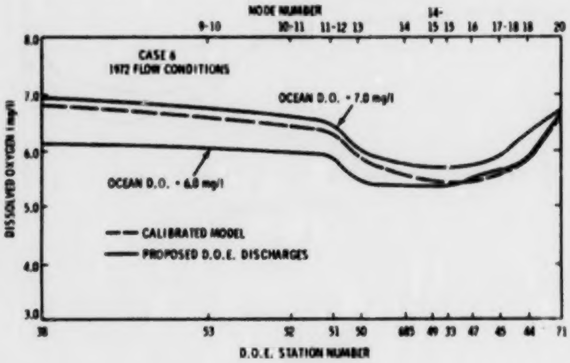

Figure 8.

Figure 9 shows the predicted results of combining the pulp mill discharges. The model predictions show virtually no difference between results of the separate and combined discharges (Figures 8 and 9).

The last alternative placed the entire industrial discharge much closer to the estuary mouth. The results for the proposed discharge levels and a benthic oxygen demand of 2.0 g/m^2/day between the discharge and the estuary outlet indicated essentially no oxygen depletion. The calculations show that for these conditions DO in the estuary may be very nearly equal to the concentration in incoming seawater. However, this result should be interpreted cautiously because there is presently no information about tidal exchange coefficients.

Study of saltwater intrusion based on 1972 hydraulic conditions showed that water similar to ocean water extends nearly up to the region of DO sag examined earlier, corroborating the small DO change up to this point.

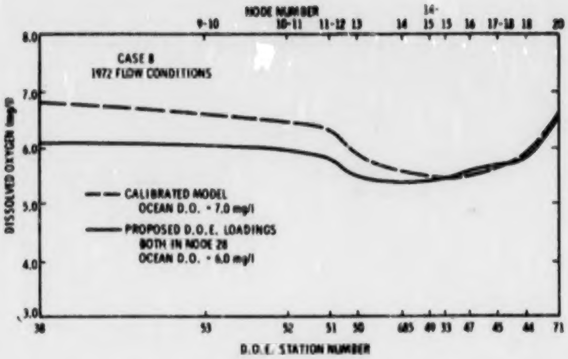

Figure 9.

MONITORING SYSTEM IMPROVEMENTS

It is suggested that future effort be devoted to field measurements of benthic oxygen uptake rates and the determination of ebb and flood tide water quality at the seaward boundary of Grays Harbor. The benthic measurements should be made in the North and South Channels and up the Chehalis River to Cosmopolis.

Other monitoring system improvements, such as the measurement of nutrient concentration and photosynthetic rates, would be valuable but of secondary importance compared to the above suggestions.

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MATHEMATICAL MODEL OF A GREAT LAKES ESTUARY

Charles G. Delos
U.S. Environmental Protection Agency
Chicago, Illinois

Abstract

A one dimensional steady state finite section estuary model was applied successfully to the lower 11 miles of the Black River of Ohio. The approach used was necessitated by the fact that water quality in the lower portion of the river is strongly influenced by Lake Erie waters. The one dimensional estuary model represents a compromise between conventional stream models, which are fundamentally inadequate to simulate this type of system, and multi-dimensional models, which require considerably greater resources to apply successfully. The approach used is likely applicable to the lower reaches of nearly all rivers tributary to the Great Lakes.

General Considerations

The Black River of Ohio drains an area of 467 square miles to Lake Erie. Water quality of the lower 11 miles of the river is severly degraded by discharges from U.S. Steel Lorain Works and the cities of Elyria and Lorain sewage treatment plants. In order to assess the degree of waste treatment required to attain acceptable levels of dissolved oxygen in the river, field data collection and mathematical modeling was initiated by U.S. Environmental Protection Agency.

The study area shown diagramatically in Figure 1, encompassed 11.3 miles of waterway, extending from above Elyria STP (River Mile 10.8) down through the river-harbor interface (R.M. 0.0), out to the harbor-lake interface (R.M. -0.5). Above approximately River Mile 6.5, the Black River is a free flowing stream. Below this point water level and quality are influenced by backwaters of Lake Erie; thus, although it is not saline, the system conforms to an accepted definition of an estuary.[1, 2] Following the last glacial retreat the stage of Lake Erie has been hypothesized to have risen significantly due to gradual upwarp of the outlet sill in response to removal of the ice loading.[1, 3] The river valley formed by downcutting during the low water period was thereby drowned, forming the present backwater.[1, 2] Additional enlargement of the lower 3 miles of channel has been done by man to expedite navigation.

While the free flowing portion of the river (R.M. 10.8 - 6.5) is shallow and of moderate velocity and slope, the estuary portion is quite deep and slow moving. Here current measurements and water quality data indicate stratification with intrusion of cleaner, cooler Lake Erie waters beneath the warmer effluent waters.

Vertical concentration gradients were not found to be excessive, however. The variation of dissolved oxygen with depth averaged about 1 mg/l in the lower portion of the river. Consequently, it is appropriate to describe the system one dimensionally using the average concentration (from top to bottom) at each station as commonly applied to pollution analysis of estuaries. In this case, the transport of material caused by the rather complex hydrodynamic behavior in the estuary portion of the river is described in terms of advective and dispersive transport along the longitudinal axis, as discussed by Harleman.[4]

The hydrograph of the Black River at Elyria indicated that a very low and relatively steady flow regime had been maintained for about two weeks preceding the July 1974 survey and continued throughout the survey period. Under such conditions, the system is likely to approach a steady state.

The mathematical description of water quality behavior in a one dimensional estuary under steady state conditions is well developed and is elucidated elsewhere.[5] Furthermore, a number of computer programs are available to expedite solution. The program utilized, the AUTO-SS version of AUTO-QUAL, incorporates a finite section approach.[6] The river, between R.M. -0.6 - 10.8 was divided into a large number of equal length segments within which mixing was assumed to be complete. Concentrations were determined by advective and dispersive transport into and out of each section and by the sources and sinks of material within each section.

For a system thus discretized the dissolved oxygen concentration in section j, located upstream of section j-1 and downstream of section j+1, is defined by

$$
\begin{aligned}
0 = {} & (-Q_j DO_{j+1} + Q_{j-1} DO_j - qout_j DO_j + qin_j DOin_j)/V_j \\
& - \left(E_j A_j \left(\frac{DO_j - DO_{j+1}}{X} \right) + E_{j-1} A_{j-1} \left(\frac{DO_j - DO_{j-1}}{X} \right) \right) / V_j \\
& - K_{C_j} CBOD_j - K_{N_j} NBOD_j + K_{A_j} (DOsat_j - DO_j) + P_j - R_j - SOD_j
\end{aligned}
$$

where

A = cross sectional area (L^2)
DO = dissolved oxygen concentration (M/L^3)
E = dispersion coefficient (L^2/T)
K_A = reaeration coefficient ($1/T$)
K_C = carbonaceous BOD decay coefficient ($1/T$)
K_N = nitrogenous BOD decay coefficient ($1/T$)
P = photosynthetic oxygen production ($M/L^3/T$)
Q = river flow (L^3/T)
qin = effluent or tributary flow (L^3/T)
$qout$ = diversion flow (L^3/T)
R = algal respiration ($M/L^3/T$)
SOD = sediment oxygen demand ($M/L^3/T$)
V = section volume (L^3)
X = section length (L)

The primary difference between the finite section estuary model and the finite section stream model (e.g., QUAL-II[7]) is that the downstream boundry condition must be fixed in order to model the estuary. This reflects the obvious fact that the water quality of Lake Erie (a large system) is relatively unaffected by conditions in the Black River (a small system).

Model Calibration

The calibration is based on a rather comprehensive field survey performed on July 23-26, 1974.

Hydraulic Characteristics

Flow conditions comparable to the once in 10 year 7 day low flow were observed in the river during the

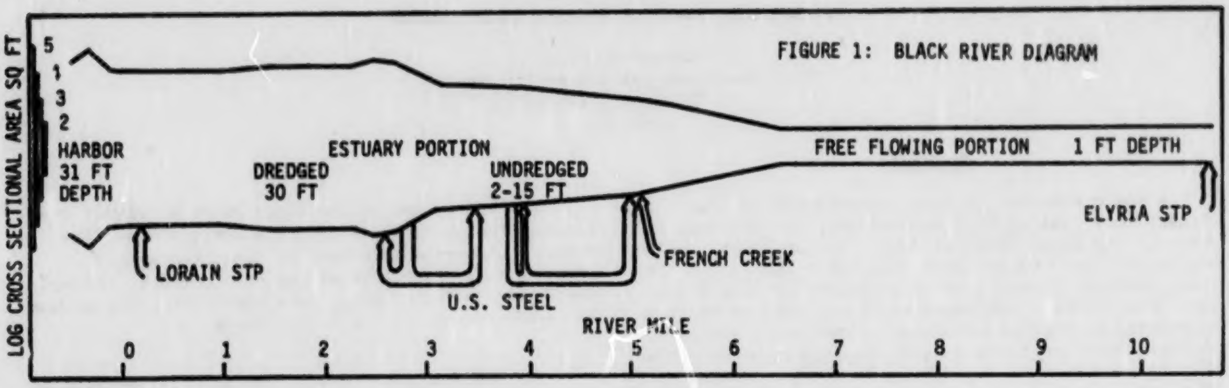

FIGURE 1: BLACK RIVER DIAGRAM

July 1974 survey. Net flow traveling past the steel mill averaged 25.4 cfs. This low flow is dwarfed by the 266 cfs cycled through the steel mill intakes and outfalls.

Hydraulic slope in the free flowing portion of the river (above R.M. 6.5) averaged 4.7 ft/mile. At R.M. 6.5 the Lake Erie water elevation essentially intercepts the river elevation and the river bed slope of 3-4 ft/mile results in increasing depth. Below R.M. 2.9, the channel is dredged to a depth of 30 ft. Channel dimensions are shown in Figure 1.

Current measurements were made at two cross sections (R.M. 2.3 and 3.1) in the estuary portion of the river. Four times in three days, current direction and velocity were measured at 3 foot depth intervals at 3-5 points along each transect. The longitudinal component of velocity, averaged laterally and temporally, is shown in Figure 2. Intrusion of lake water beneath the effluent waters is clearly indicated in both cases. Flow was more sharply stratified at the more upstream cross-section. Also noteworthy at this cross-section is the small current traveling downstream along the river bed, possibly originating from cool upstream water which escaped entrainment in the upstream water intake.

The net advective velocity, computed for the simulation from flow and channel dimensions, was only 0.02 and 0.001 ft/sec at the upper and lower cross sections respectively. These very low velocities sharply contrast the maximum stratified current velocities (shown in Figure 2) of 0.25 and 0.2 ft/sec at the upper and lower cross sections respectively. The necessity for a high degree of longitudinal dispersion in a one dimensional model is thus apparent.

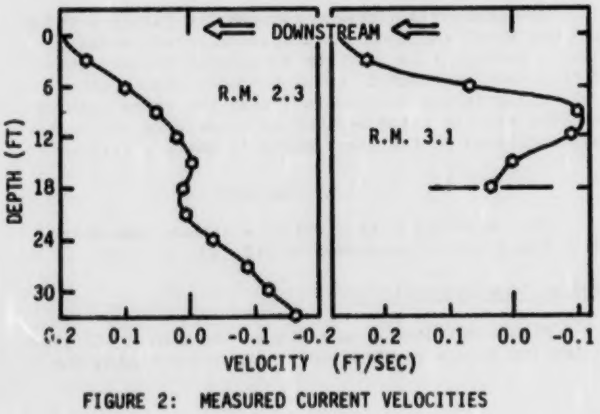

FIGURE 2: MEASURED CURRENT VELOCITIES

The longitudinal dispersion coefficient, E, was determined from conservative materials profiles, using the trial and error fit procedure described by Thomann for use with finite difference computation.[5] The value of E is shown as a function of river mile in Figure 3. Comparison of observed and predicted dissolved solids profiles is shown in Figure 4. Fluoride, chloride, and sulfate displayed analogous profiles and comparable fits.

The observed level of dispersive mixing is believed to be a manifestation primarily of the stratified flow conditions which result from gravitational instability of the lighter effluent waters and heavier lake waters. The 3-4 °C vertical temperature differentials represent density differentials of approximately 0.001 g/ml. It is also likely of importance that the steel mill withdraws water from some distance beneath the surface and discharges heated effluent at the surface. The dispersion coefficient, highest below the steel mill, decreases in the harbor towards values expected for near shore and open lake waters.

Wind effects, in the form of seiches, may also constitute a portion of the dispersive energy. Lunar tides, on the other hand, are not observed on the Great Lakes.

Dissolved Oxygen Balance

Reaeration capacity, K_A, was calculated using the O'Connor formula modified as recommended by O'Connor:[8,9]

$$K_A = K_L/H$$

and $$K_L = 12.9\ U^{1/2}/H^{1/2}$$

constrained by $K_L \geq 2$

where K_L is the surface transfer coefficient, H is depth, and U is net velocity.

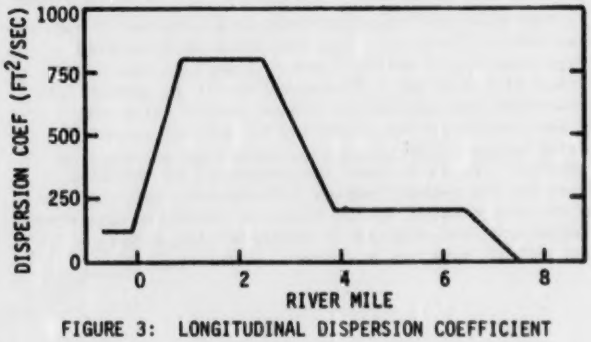

FIGURE 3: LONGITUDINAL DISPERSION COEFFICIENT

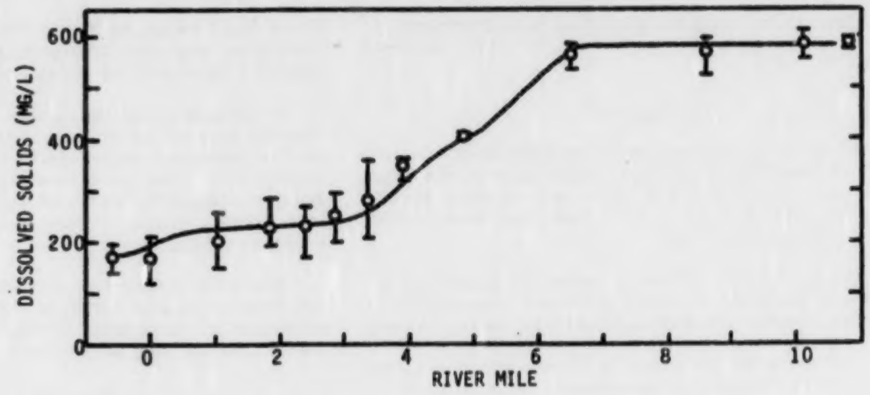

FIGURE 4:

OBSERVED AND PREDICTED
DISSOLVED SOLIDS
JULY 23-26, 1974

The Tsivoglou formula[10] was considered for application to the free flowing portion but was found to significantly underestimate reaeration capacity. The Churchill formula, on the other hand, was considered to be inapplicable for this situation as it was developed for streams with velocities considerably higher than found anywhere in the study reach, and depths greater than those found in the free flowing portion.[11] Its use would also underestimate reaeration capacity.

The bulk of the oxidizable nitrogen consisted of ammonia. As the rate limiting step under this condition can be expected to be ammonia oxidation, a single first order kinetic reaction will closely approximate the three or four stage reaction (depending on whether starting with ammonia or organic nitrogen):[8, 12]

$$\text{Org-N} \rightarrow NH_3 \rightarrow NO_2 \rightarrow NO_3$$

Nitrogenous BOD (NBOD) was calculated based on total Kjeldahl nitrogen concentration.

Differences in decay rates were expected to exist between the estuary and free flowing portions of the river, due to differences in benthal character, ratio of volume to benthal surface, and rate of replacement of fluid elements at the benthal interface.[8] In the free flowing portion (above R.M. 6.5) the decay coefficient was found to be 0.15 day^{-1} (base e) based on the observed rate of disappearance. Such a low rate is characteristic of a system dominated by gross levels of carbonaceous BOD.[8]

The decay coefficient in the estuary portion of the river was estimated to be 0.05 day^{-1}, based on fit to the observed NBOD levels. This unusually low rate is attributed to insufficient levels of dissolved oxygen existing through much of the estuary.[8, 9, 12]

Carbonaceous BOD (CBOD) was determined from the long term BOD (20 or 30 day BOD) less the NBOD. The decay coefficient, estimated from observed CBOD levels and rates of disapperance, was found to be 0.7 day^{-1} in the first mile below Elyria STP, 0.5 day^{-1} through the remainder of the free flowing portion of the river, and 0.14 day^{-1} in the estuary portion.

BOD loading is summarized in Table 1.

Table 1: Oxygen demanding effluent loads (lbs/day)

Source	CBOD	NBOD
Elyria STP	9800	5000
U.S. Steel (net)	14000	8700
Lorain STP	2600	2800

The diurnal dissolved oxygen variation at all stations in the estuary portion of the river was either small or inconsistant with photosynthetic activity. Negligible algal productivity is likely a consequence of rapid light extinction in the water column.

Sediment oxygen demand (SOD) measurements were made at various locations. When converted to mg/l/day, the SOD was found to be minor relative to the oxygen uptake of BOD dissolved and suspended in the water column ($K_C \times \text{CBOD} + K_N \times \text{NBOD}$, in mg/l/day).

Thus, without incurring significant error, the accumulation of organic matter in the sediments could be assumed to have attained a steady state, with the rate of decay within the sediments balanced by the rate of deposition.[13] The small sediment oxygen demand found was therefore implicitly accounted for in the BOD decay, as originally suggested by Streeter.[14]

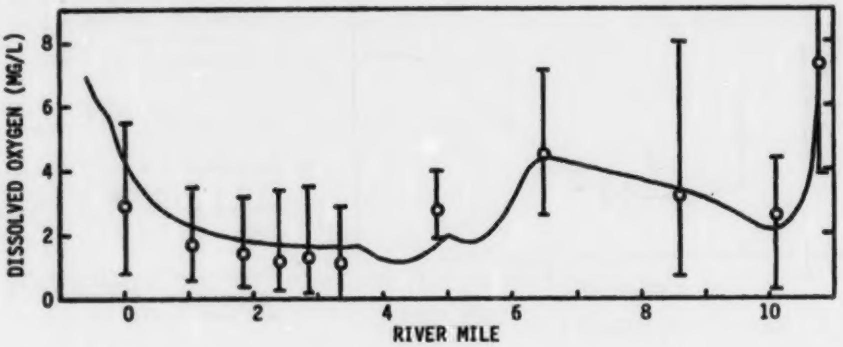

FIGURE 5:

OBSERVED AND PREDICTED
DISSOLVED OXYGEN
JULY 23-26, 1974

Comparison of observed and predicted dissolved oxygen concentrations for the July 1974 survey is shown in Figure 5.

Verification

Water quality data collected in September 16, 1975 was used to test the predictive capability of the model. Net flow past U.S. Steel was approximately four times greater, and temperatures 3-4 °C less than those found during the July 1974 survey.

As the U.S. Steel effluents were not monitered at this time, previously measured net loads (concentration deltas between intakes and outfalls) were assumed. However, due to the high degree of recirculation through the river by the steel mill, the plant's intake and effluent qualities are interdependent upon each other. Subsequent to using a tedious manual convergence method involving several computer runs to determine the correct intake and outfall concentrations for a given set of conditions, the computer program was modified to couple each intake to the outfall it feeds (as shown in Figure 1). Effluent BOD was computed from the given change in BOD between intake and outfall, added to the intake BOD computed during the previous iterative step in the solution.[15]

Effluent dissolved oxygen (DO) was handled in analogous manner; however, the relationship between the intake and outfall DO is more complex. The following simplification of the process is expected:

(1) Water is pumped from intake with DO concentration C_i.

(2) Temperature is raised to outfall temperature; DO saturation is depressed to CS_o; deficit is $D_i = CS_o - C_i$.

(3) Water undergoes reaeration in returning to lake elevation, resulting in new deficit D_o: $D_o/D_i = e^{-K_A t}$, where K_A is a reaeration coefficient.

The product $K_A t$ (or ratio D_o/D_i) was determined from the July 1974 data. Since the reaeration coefficient can be expected to be temperature dependent, an Arrhenius rate dependency was assumed.

Comparison of observed and predicted dissolved oxygen concentrations for the September 1975 survey are shown in Figure 6.

Sensitivity Analysis

The sensitivity of dissolved oxygen predictions to changes in system parameters under low flow conditions was investigated. The analysis was based on conditions expected following implementation of improved treatment by dischargers.

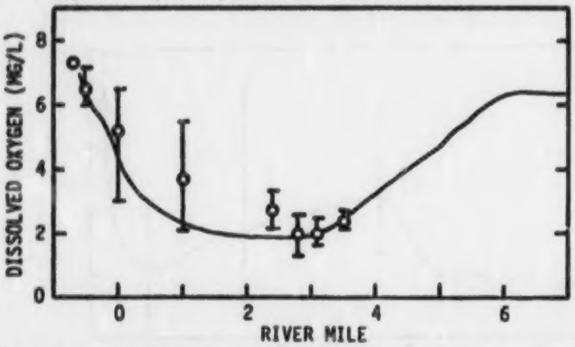

FIGURE 6: OBSERVED AND PREDICTED DO, SEPT. 16, 1975

Predicted dissolved oxygen levels were most sensitive to changes in the reaeration and dispersion coefficients and Lake Erie BOD (downstream boundary condition). They were less sensitive to CBOD and NBOD decay coefficients and Lake Erie dissolved oxygen, and were quite insensitive to river flow and upstream boundary conditions.

The great difference in sensitivity to dispersion and flow of course reflects the previously discussed magnitude of difference between stratified flow velocities and net advective velocity.

Conclusion

Intrusion of Lake Erie waters into the Black River estuary is brought about primarily by thermally induced density differences between Lake and effluent waters. Under low flow conditions net advection downstream plays little role in the transport of pollutants out of the estuary. Rather, transport brought about by opposing vertically stratified flows may be simulated as longitudinal dispersion in a one dimensional, steady state estuary model. The magnitude of the dispersion coefficient used is somewhat smaller than found for many ocean estuaries, but greater than normally applied to streams or lakes.

The approach taken is adequate for planning and enforcement purposes.

Additionally, due to the sluggish flow in the backwater, reaeration is best calculated from basic surface transfer considerations (surface to volume ratio), with minimum values of surface transfer coefficient chosen independently of flow turbulence (velocity, depth, slope) considerations.

The observed influence of the lake on water quality in the lower reaches of the river also has an important implication to the modeling of Great Lakes. Loads to Lake Erie calculated by multiplying the observed concentration by the net advective flow will significantly underestimate the true load being delivered to the lake (by dispersive transport). Using concentrations observed further upstream will by-pass this effect but will also fail to include major waste sources.

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COST-EFFECTIVE ANALYSIS OF WASTE LOAD ALLOCATIONS

John Kingscott, Environmental Protection Agency, Washington, D.C.

Introduction

The Federal Water Pollution Control Act Amendments of 1972 require the States to identify those waters for which the minimum legislated effluent limitations are not stringent enough to meet applicable water quality standards. Roughly 2000 segments have been identified as being water quality limited for a variety of reasons. The waste load allocation procedure is used to determine effluent limitations based on water quality considerations rather than uniform applications of technology. State Basin Planning under Section 303 of the Act and currently Water Quality Management Planning under Section 208 is attempting to ensure that the 1983 goals of fishable and swimmable water uses will be achieved in these segments. The potential investment of large sums of money for advanced waste treatment justifies a close look at the practical implications of the waste load allocations. Much of the current attention being given to nonpoint sources is the result of a concern that these sources will negate the upgrading of water uses despite increased levels of point source control. However, many segments do have predominately point source problems or the nonpoint problems can be independently addressed for periods of high flow.

Common stream analysis practice consists of the application of verified deterministic models to predict the water quality response during critical or design conditions. The behavior of any water segment can most reasonably be approximated as a probabilistic system since the flow, temperature, waste load, and initial instream concentrations all vary over time. The state of the art in model development is far beyond the availability of basic data and insight into biological processes needed to broadly apply more sophisticated methods. This emphasizes the need for judgment in interpreting the results of the simpler deterministic models.

This paper considers the relative consequences of some procedures used in the application of deterministic models, in particular the choice of design conditions and seasonal application of waste load allocations. It was desired that the analysis be general and applicable to a number of situations and issues. It was also necessary not to be hypothetical but to address real situations. The resulting analysis considers the costs of advanced waste treatment and the effects in terms of a risk for the violation of dissolved oxygen stream standards. An effluent analysis was undertaken to define an empirical procedure for generating effluent loading factors. The waste treatment costs were considered by combining flow dependent unit processes to form viable treatment systems. Five water quality limited segments were analyzed using historical U. S. Geological Survey streamflow records. Cost-effective curves were generated to define feasible treatment options for nitrogenous and carbonaceous BOD removal. The optimal investment strategy for levels of treatment higher than secondary was then used to study issues related to waste load allocations.

Effluent Analysis

A number of factors can be expected to affect treatment efficiency and the variability of effluent loadings. The need existed to produce a generally applicable procedure to generate BOD loadings for different treatment schemes.

Daily effluent BOD concentrations were analyzed for nine Michigan and five Texas[3] secondary plants. The mean, variance, and coefficient of skewness were obtained for one year of operation of each of the plants. The distributions were assumed to be log normal and a method was sought to generate synthetic daily mean concentrations given an annual mean effluent load.

Matalas[6,4] has suggested a procedure for preserving the moments of a distribution when log values are generated. If "a" is the lower bound of random daily BOD represented by χ, then $y = \log(\chi - a)$ is normally distributed. If the χ parameters represent the daily mean concentration of BOD, they are related to the y parameters as follows:

$$\mu(x) = a + \exp\left[\sigma^2(y)/2 + \mu(y)\right] \quad (1)$$

$$\sigma^2(x) = \exp\{2\left[\sigma^2(y) + \mu(y)\right]\} - \exp\left[\sigma^2(y) + 2\mu(y)\right] \quad (2)$$

$$\gamma(x) = \frac{\exp\left[3\sigma^2(y)\right] - 3\exp\left[\sigma^2(y)\right] + 2}{\{\exp\left[\sigma^2(y)\right] - 1\}^{3/2}} \quad (3)$$

where μ is the mean, σ^2 is the variance, and γ is the coefficient of skewness.

To preserve the statistics of the generated BOD values, the mean, variance, and coefficient of skewness are determined for the historic distribution (the χ variables); substituted into equations 1, 2, and 3; and solved for $\mu(y)$, $\sigma^2(y)$ and "a." These are the parametric values that are used in the generation process to give a series of synthetic normally distributed logarithms $y_1, y_2 \ldots y_n$. The generated BOD's are then calculated back through the transformation by the relation:

$$x_i = \exp(y_i) + a$$

The independent variables chosen to describe the distribution were the wastewater discharge Q, in mgd, and yearly average effluent BOD concentration $\mu(\chi)$ in mg/l. The following empirical relationships were developed by stepwise regression:

$$\sigma^2(\chi) = 4.06\ \mu(\chi)^{1.27} Q^{-.25} \quad (4)$$

multiple correlation coefficient = .83

$$\gamma(\chi) = 5.81\ \mu(\chi)^{-.43} \quad (5)$$

multiple correlation coefficient = .47

Thus normally distributed logs could be generated and transformed into daily mean concentrations of effluent BOD. The standard deviations for distributions thus generated are related to those for the historical operation of the treatment plants in figure 1. The response of the generated distributions to variations of the independent variables is given in figure 2.

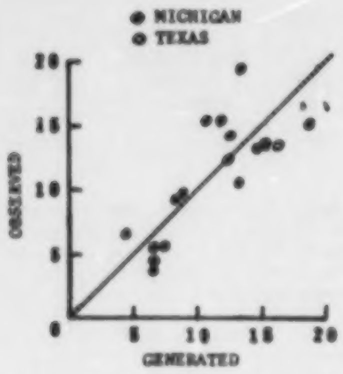


Fig. 1. Comparison of generated and observed standard deviations.

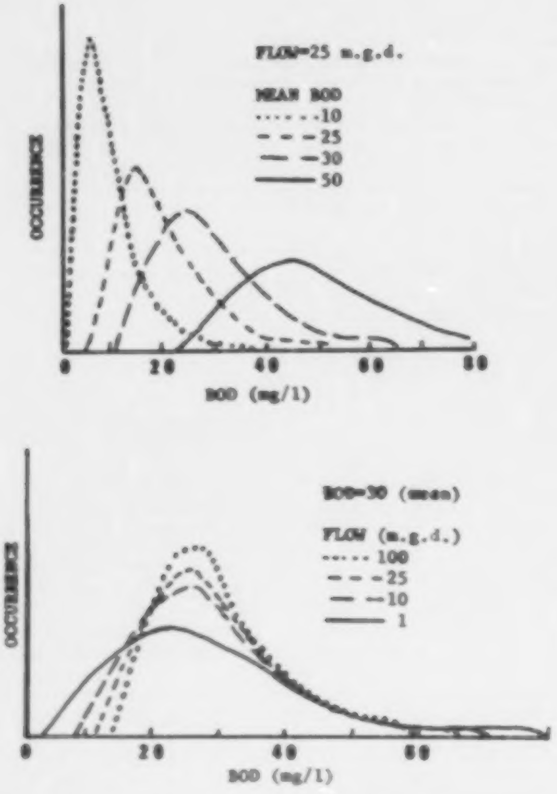


Fig. 2. Response of the generated BOD distribution to changes in waste flow and mean BOD.

This technique serves as a crude approximation of reality and does not consider numerous important factors. However, the procedure is very general and can be applied with a minumum amount of information.

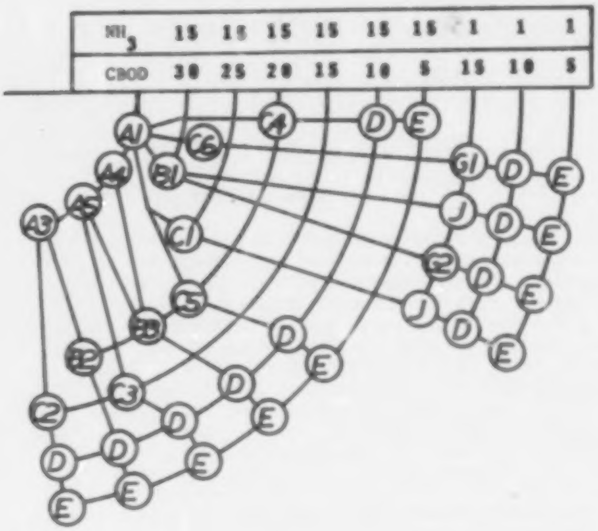
Cost Analysis

Costs were calculated using combinations of various unit processes for wastewater treatment and sludge disposal.[10] Consideration was given to those processes which remove oxygen demanding material for what might be considered secondary and advanced systems. The various combinations of processes were classified according to characteristic effluent quality assuming a typical influent waste stream. Compatible unit processes were combined as building blocks considering basic design criteria, equipment sizing, and quantities and characteristics of sludges so that compatible combinations were formed.

The total cost for each unit process was determined based on wastewater flow and includes capital, operation, and maintenance. These costs were developed based on unit sizing as determined by standard design criteria, process loading capabilities, solids generation, chemical and energy consumption, and manpower requirements. The values were trended to a common cost level representative of February 1973. Figure 3 traces the combinations of unit wastewater processes and the effluent values which are characteristic of the combined systems.

Figure 3

WASTEWATER TREATMENT
UNIT PROCESS COMBINATIONS



A1 CONVENTIONAL PRIMARY
A3 PRIMARY WITH SINGLE STAGE LIME ADDITION
A4 PRIMARY WITH ALUM ADDITION
A5 PRIMARY WITH FERRIC CHLORIDE ADDITION
B1,2,3 TRICKLING FILTER
C1,2,3 ACTIVATED SLUDGE
C4 ACTIVATED SLUDGE WITH ALUM ADDITION
C5 ACTIVATED SLUDGE WITH FERRIC CHLORIDE
C6 HIGH RATE ACTIVATED SLUDGE
D FILTRATION
E ACTIVATED CARBON
G1,2 BIOLOGICAL NITRIFICATION
J BREAK POINT CHLORINATION

Segment Analysis

The fundamental equation which describes the longitudinal distribution of dissolved oxygen can be developed from the principles of mass balance and continuity. An advective system with carbonaceous and nitrogenous oxygen sinks and first order kinetic relationships takes the following form:

$$\frac{\partial C}{\partial T} = -\frac{1}{A}\frac{\partial}{\partial X}(QC) + K_s(C_s - C) - K_d L(x) K_n N(x) \quad (6)$$

where:
C = concentration of dissolved oxygen
C_s = saturation concentration of D.O.
K_a = reaeration rate constant
K_d = carbonaceous BOD oxidation rate constant
$L(x)$ = concentration of carbonaceous BOD
K_n = nitrogenous BOD oxidation rate constant
$N(x)$ = concentration of nitrogenous BOD
Q = river volumetric flow
A = river cross-sectional area
x = longitudinal distance

Equations of this nature have been solved by Li[5] for the case where boundary conditions are arbitrary functions of time and by DiToro and O'Conner[2] for the case where boundary conditions are functions of time and the flow is time-variable. The steady state solution to equation 6 for constant boundary conditions and coefficients is:

$$D(x) = C_s - C(x) = D_o \exp^{-K_a \frac{x}{u}} + \frac{K_d L_o}{K_a - K_d}\left[\exp^{-K_d \frac{x}{u}} - \exp^{-K_a \frac{x}{u}}\right] + \frac{K_n N_o}{K_a - K_n}\left[\exp^{-K_n \frac{x}{U}} - \exp^{-K_a \frac{x}{U}}\right] \quad (7)$$

where:
$D(x)$ = distribution of D.O. deficit
D_o, L_o, N_o = initial concentrations
$u = Q/A$ = stream velocity

Historical daily streamflows were considered along with randomly generated waste loads and characteristic monthly temperatures to calculate a minimum dissolved oxygen value with equation 7. This method implies that the stream flow and velocity are constant for one day and then abruptly change to another constant value the subsequent day and so on. It is important to note that equation 7 describes a profile derived from steady state conditions for constant streamflow, waste load, and reaction rate coefficients. However, the equation was applied by assuming the parameters are constant for one day and then immediately change. Limitations to this approach[1] imply that the solution is valid only for one day's travel time below the waste source. This will be significant for relatively small reaction rate coefficients which cause the minimum D.O. to occur some time after one day from the time of input. The significance of this fact on the analysis is unknown but could conceivably be small if D.O. standards violations are occurring during relatively steady flow periods on the recession tail of the hydrograph.

Five stream segments that are water quality limited for dissolved oxygen were analyzed. The segments have been modeled through the EPA National River Basin Modeling Program and represent a variety of hydrologic conditions.

Segment	State	Basin	Average Flow (cfs)
Flint	Ga.	Chattahoochee	345
Cache La Poudre	Colo.	S. Platte	130
Schuylkill	Pa.	Delaware	1740
Reedy	S.Car.	Santee	85
Upper Miss.	Minn.	Mississippi	12090

The stream hydraulic descriptions were simplified and assumed to be constant for the entire segment. Municipal and industrial waste sources were combined for the simulation so either one or two point sources were included depending on the existence of industrial discharges. The distribution of daily loadings for an industrial source was assumed to have the same characteristics as a municipal source but generated independently. The nitrogenous BOD component was assumed to also have the same log normal characteristics.

U. S. Geological Survey stream gaging stations exist on all segments, and daily flows for the last twenty years of record were obtained from STORET (except the Colorado stream where twelve years are available). The daily stream flows were used to calculate the hydraulic response and the reaeration rate constant. Daily waste loadings were produced by assuming a constant waste flow and randomly generated daily mean concentrations. Consequently, the loadings were assumed to be independent of the time of year and streamflow. Representative monthly water temperatures were determined from the U. S. Geological Survey Water Resources Data-Water Quality Records. Representative boundary conditions were determined from the original model validation studies and assumed to be constant. The power functions for velocity, depth, and reaeration coefficient determination and reaction rate constant temperature adjustments were applied over the wide range of flows and temperatures. Table I shows the values which were used for the simulations.

The simulation procedure was used to calculate the cost-effective curves unique to each segment system shown in figure 4. For each classification of effluent quality a simulation was made from the historical daily streamflow records to determine the number of times the average daily oxygen was below a standard of 4 mg/l. This standard has tentatively been identified[8] as providing a low level of protection; that is, it should permit populations of tolerant species and successful passage of most migrants while there may be a reduced production or elimination of sensitive fish. The corresponding costs were determined as the least costly combination of unit processes capable of achieving the effluent values (including sludge disposal). The ammonia removal points were determined by considering an average of four alternatives--trickling filter and break point chlorination, trickling filter and biological nitrification, activated sludge and break point chlorination, and high rate activated sludge with biological nitrification. The averaging was done to generalize the procedure as biological nitrification was less costly but potential seasonal operating problems and perhaps land requirements would not always make it the more reasonable choice. Ammonia removal was considered on increments of one quarter of the waste flow to aid the construction of a continuous plot. This possibility is not unreasonable and might be compared to split treatment in a water softening operation. The resulting cost-effective curves provide a guide to the selection of advanced treatment schemes that minimize the total cost associated with a given frequency of oxygen standard violation. The curves map the optimal

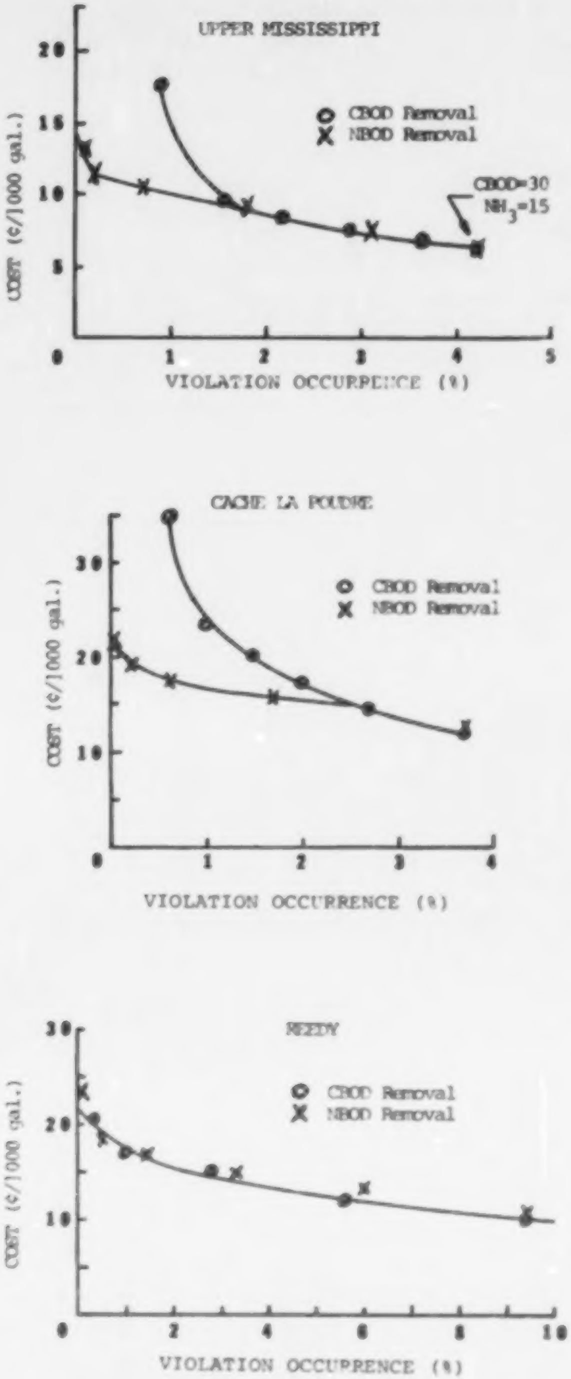


Fig. 4. Cost-effective curves for three river segments.

choice of advanced treatment schemes and clearly define the point at which ammonia removal should be considered. In some segments there is a strong indication that an understanding of the process of stream nitrification is important to waste load allocation decisions and efforts should be made to assess the likelihood of its occurrence.[9,10] The adequacy of first order kinetic relationships should probably also be confirmed against possible nonlinear approaches that may more reasonably represent the autotrophic bacteria activity.

Waste Load Allocation Analysis

The implications of a seven-day ten-year low flow for allocations have been questioned as the practice is based on tradition rather than substantive justification. The effects of the choice of alternative critical conditions and vary'ng modes of operation deserve further investigation.

For each of the five segments a 3% annual growth rate was assumed and allocations calculated for a twenty-year flow projection. Seven-day two-, five-, and ten-year low flows were calculated from the historical record and allocations determined with the maximum monthly temperature. The occurrence of oxygen violations and corresponding total costs for secondary treatment (carbonaceous BOD = 30 and ammonia = 15) and low flow dependent allocations under present waste flow conditions are given in figure 5. The occurrence is expressed as a percent and calculated by dividing the number of days having a mean D.O. below 4.0 mg/l. by the number of historical daily average flows. The segments show varying degrees of sensitivity to the choice of critical flow conditions.

The increased liklihood of an instream violation as point source flows increase to the twenty-year projected level while concentrations are held constant is given in figure 6. Simulations were also made at the twenty-year projected flow with the carbonaceous reaction rate decreased by 25% as an indication of a possible safety factor resulting from a biologically more stable waste from advanced treatment processes.

The result of adherence to the load allocation for specified months of the year is shown in figure 7. A four-month effluent standard (July, August, September, & October) and six-month standard (June, July, August, September, October, & November) are compared to yearly operation at the allocated level. The Georgia

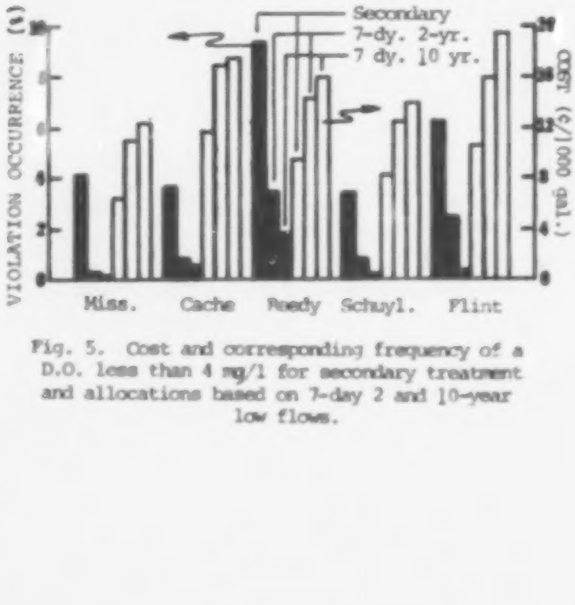


Fig. 5. Cost and corresponding frequency of a D.O. less than 4 mg/l for secondary treatment and allocations based on 7-day 2 and 10-year low flows.

TABLE I

Values of Constants and Boundary Conditions used for Simulation

SEGMENT	Municipal Flow (mgd)	Industrial Flow (mgd)	Velocity (ft/sec)	Depth (ft)	K_2 (dy^{-1})	K_d (dy^{-1})	K_n (dy^{-1})	Initial CBOD (mg/l)	Initial NH_3 (mg/l)
Upper Mississippi	250	0	.000133Q	10.7	$\frac{12.96u^{.5}}{D^{1.5}}$	.35	.1	2	.25
Reedy	15	7	$.038Q^{.716}$	$.292Q^{.412}$	$\frac{7.6u}{D^{1.33}}$	.6	.03	3	.2
Schuylkill	25	-	$.06Q^{.4}$	$.8Q^{.23}$	$\frac{7.6u}{D^{1.33}}$	.55	.2	3	1.0
Cache La Poudre	7	6	$.0855Q^{.17}$	$.44Q^{.335}$	$\frac{2.833u}{D^{1.5}}$	.5	.4	3	.25
Flint	10	1	$.09Q^{.31}$	-	$\frac{.45\Delta h}{tf}$	.4	.5	2	0.0

Q = streamflow, in cfs
Δh = change in water surface elevation, in feet
tf = time of travel, days
D = mean depth of stream, in feet
u = mean velocity of stream, in ft/sec

and South Carolina segments show some difference between four- and six-month standards, while the Minnesota and Pennsylvania streams exhibit the practicality of a four-month requirement. The capital and annual operation and maintenance costs for secondary and the increment for advanced treatment are given. Relative to secondary treatment, a greater proportion of the total cost associated with the load allocation is for operation and maintenance. This is due in part to the higher cost of operating break point chlorination which was averaged with biological nitrification to form the means of ammonia removal.

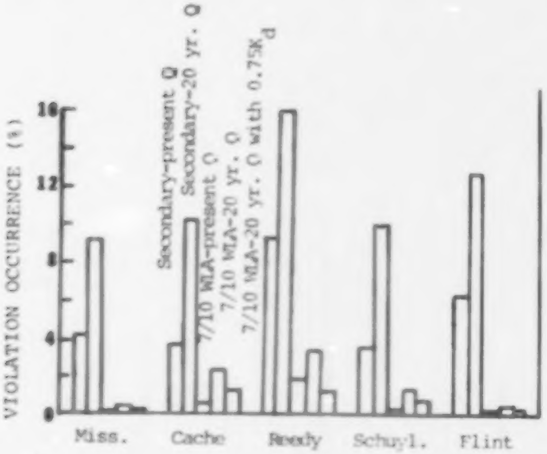


Fig. 6. Frequency of a D.O. less than 4 mg/l at present wastewater flow and 20 year projection at a 3% increase per year.

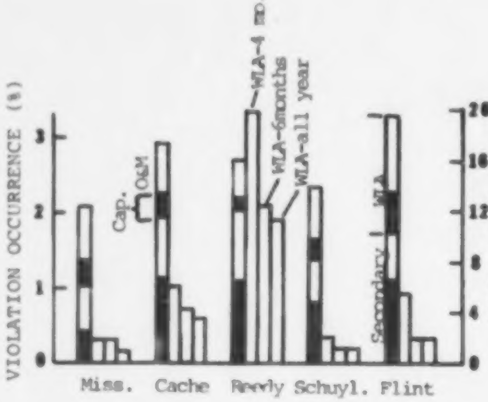


Fig. 7. Amortized capital costs and annual operation and maintenance costs for a 7-day 10-year WLA and corresponding instream violations for time dependent operation.

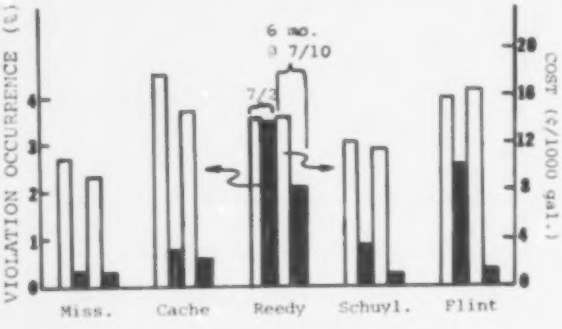


Fig. 8. Costs and instream D.O. violations for 7 day-2year allocation and 6 months operation at 7-day 10-year allocation.

Figure 8 is a comparison of seven-day two-year based effluent limits with seven-day ten-year based limits which are practiced for six months with secondary treatment the remaining months. The costs for the seasonal treatment option were calculated by assuming the operation and maintenance costs for the advanced treatment processes were less by one half for six months of operation. The figure shows the advantage of a seasonal effluent limit for all segments.

Conclusions

The assumptions made in this analysis imply that the absolute values for the cost and violation occurrence are of secondary importance to their relative values. Assuming the existence of a verified deterministic stream model the procedure given may be used to produce cost-effective curves which guide the choice of advanced wastewater treatment schemes. With the minimum legislated levels of treatment it is probable that stream nitrification will become increasingly important and should be given close attention during model calibration and verification. The waste load allocation procedure is an effactive means for controlling the risk of a stream standards violation and absorbing the effects of increased waste flow. In some segments the significant difference in the risk associated with the two-year and ten-year recurrence interval for the design condition indicates the advantage of using the more stringent requirement. Cost-effective considerations imply the practicality of implementing variable effluent limits such as on a seasonal basis.

This work was stimulated by practical concerns. The assumptions made were necessary to produce results which could provide some insight into policy decisions which must be made soon due to legislated deadlines. Additional work is needed to assess the implications of the various application-oriented procedures and decisions which must be addressed by those involved with all phases of related water quality planning.

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WASTE ALLOCATIONS IN THE BUFFALO (NEW YORK) RIVER BASIN

Donald H. Sargent
Versar Inc.
Springfield, Virginia

Abstract

A water quality simulation model, VERWAQ, was developed for the complex hydraulic and waste load characteristics of the Buffalo River. These characteristics include very low water velocities, oscillating flow, upstream flow, inter-basin transfer of water, many critical conservative and non-conservative water quality parameters, thermal pollution, and important non-point as well as point sources of wastes. The developed and verified model was used to project water quality and to allocate waste loads.

Description of the Study Area

The Buffalo River was the subject of a comprehensive evaluation of waste loadings and water quality, performed by Versar Inc. in 1973 (under EPA Contract 68-01-1569) as part of the U.S. Environmental Protection Agency's commitments to abate and control water pollution under the 1972 Great Lakes Water Quality Agreement between the U.S. and Canada.[1] This river in western New York was identified as one of several concentrated areas of municipal and industrial activity which have had poor water quality and which contributed to the waste loads of the Great Lakes.

The Buffalo River discharges into the easternmost end of Lake Erie, just at the head (southern) end of the Niagara River. It extends only 13 kilometers (8 miles) upstream from its mouth, and is located in the City of Buffalo and in surrounding Erie County. The watershed of the Buffalo River and its three tributaries (Cazenovia Creek, Buffalo Creek, and Cayuga Creek) is roughly triangular in shape, extending to the south and east of Buffalo, and has a drainage area of 446 square miles. Except for a few miles just above their confluence with the Buffalo River, the tributaries are fast-flowing streams with primarily agricultural drainage areas and with several small communities. The lower reach of Cayuga Creek passes through the large urban residential communities of Lancaster and Depew, and bears little resemblance to its upper reaches or to the other two tributaries.

Buffalo River itself is characterized by heavy industrial development in the midst of a large municipality. Its waste load and water quality problems dominate any such concerns for the entire watershed. There are 43 individual industrial discharges into the Buffalo River. Very heavy waste loads into this reach are imposed by frequent overflows, from numerous outfalls, from the combined storm/sanitary sewer system. The problems are aggravated by the hydraulic characteristics of this reach and by large heat loads. As a result, the water quality deficiencies in the Buffalo River were (until recently) typified by a summertime dissolved oxygen concentration of less than one mg/l and by the almost complete absence of aquatic life.

Characterization of Present Conditions

Hydraulics of the Buffalo River

The industrialized reach of the Buffalo River is maintained as a shipping channel to a depth of 6.7 meters (22 feet), and has a very low slope, less than 0.2 meters per kilometer. Most of the river's volumetric flow is due to industrial discharges whose intake source is not the River but in the Buffalo Outer Harbor. These industrial flows amount to more than twice the natural discharge at average summertime conditions and to twenty times the natural discharge at critical flow conditions; resulting in a relatively stable total flow rate in summertime. Because of the very large man-made river cross-section, however, the calculated average velocity is very low, less than 0.02 meters per second, and the calculated residence time in this short reach is greater than five days.

Oscillating flow in the upstream as well as downstream direction (driven by oscillations in the level of Lake Erie) of significantly higher velocities than the calculated average, was observed and measured in the industrialized reach of the Buffalo River. Independent sets of time-varying water-level data for Lake Erie at the mouth of the Buffalo River and for the Buffalo River itself also exhibited significant oscillations. A dynamic analysis, which converted observed water level oscillations to flow rate oscillations, resulted in a calculated R.M.S. velocity of 0.096 m/sec, which is in general agreement with the R.M.S. velocity (from direct measurements of velocity) of 0.082 m/sec, and which is five times the calculated time-average downstream velocity of 0.018 m/sec. An extension of the dynamic analysis resulted in a calculated longitudinal movement of water of ± 200 meters superimposed upon the time-average movement.

Water Quality

Except for the lower reach of Cayuga Creek and for the short Buffalo River itself, most of the Buffalo River watershed (including all of Buffalo Creek and the upper reaches of Cayuga Creek) is typified by good water quality. This is consistent with an agricultural, wooded, and vacant land use pattern, dotted with small residential communities and scattered park and recreational areas.

Table 1 summarizes the water quality data for the industrial (dredged) reach of the Buffalo River. Specific contraventions of water quality standards in this reach are an average summertime dissolved oxygen concentration of 0.9 mg/l (compared to the minimum allowable of 3.0 mg/l) and an average iron concentration of 3.1 mg/l (compared to the maximum allowable of 0.8 mg/l). Although many of the other parameters, including temperature, are at high levels compared to the natural waters, no other specific water quality contraventions were found.

Chemical analysis of bottom deposits from the industrialized reach of the Buffalo River indicate high levels of oxygen demand, oil, grease, and iron. Biological sampling of these bottom deposits indicate that this reach of river is essentially devoid of bottom organisms; a finding consistent with the measured dissolved oxygen level of less than 1 mg/l.

Waste Loads

The Buffalo River receives the waste loads of its upstream tributaries, a very heavy concentration of industrial discharges, and frequent overflows from combined sewers.

The waste load to the Buffalo River from the three upstream tributaries is based upon the measured water quality and flow data for these tributaries under two conditions of flow: the average summertime flow, equivalent to the 70 per cent duration point; and the minimum average seven-day critical discharge with a recurrence interval of ten years (MA7CD/10), equivalent to the 99 per cent duration point, and specified as critical flow by the New York State Department of Environmental Conservation. The heat flux of the upstream discharge is defined as zero, with the choice of a baseline temperature equivalent to the temperature of this discharge (19.0°C in summer).

The waste load from industrial point discharges is based upon NPDES permit applications on file at EPA Region II as of July 1973. The dissolved oxygen content of the industrial discharges, not included in the NPDES permit applications, was based upon data independently supplied by the major dischargers. The heat flux was calculated from the temperature difference between each industrial effluent and the baseline temperature.

The combined sewer overflows into the Buffalo River were, for the purposes of this study, judged to be quite evenly distributed in time and in distance. Overflows from the Buffalo combined sewer system occur on the average of once every five days, and are quite evenly distributed over the year. There are 70 overflow outfalls from more than 250 overflow chambers. The fact that much of this waste is deposited on the bottom of the industrialized reach of the Buffalo River and affects water quality as a benthal load is further justification for approximating the combined sewer waste load as a distributed (non-point) load. This combined sewer overflow waste load was quantified from two studies of overflow quantity in Buffalo, from the difference between runoff and influent at the sewage treatment plant, and from two studies which characterized the constituents of combined sewer overflows in places other than Buffalo.

A comparison of the various waste loads at average summer flow, using BOD-5 as the parameter of comparison, indicates that the combined sewer overflow accounts for 31 per cent of the wastes to the Buffalo River.

Simulation Model

In general, the widely-used steady-state uniform flow stream models, which are essentially computerized versions of the Streeter-Phelps analysis for the BOD-DO relationship, are limited to the very simplest applications of point sources of wastes to a constant-temperature, non-dispersive, free-flowing stream. VERWAQ, a computerized model, was developed by extending the capabilities of existing models to accomodate the complex nature of the industrialized reach of the Buffalo River.

Features of VERWAQ

Hydraulics. The industrialized reach of the Buffalo River exhibited longitudinally homogeneous water quality measurements of virtually every parameter. The independent measurement and analysis of oscillating flow in the upstream as well as the downstream direction (driven by oscillations in the level of Lake Erie) strengthened the hypothesis that this reach may be a well-mixed body of water as opposed to a free-flowing stream. The simulation model therefore was required to test this hypothesis; e.g., VERWAQ is useful as either a plug-flow model (no longitudinal dispersion) or a completely-mixed model (complete dispersion of all constituents including heat). The same VERWAQ computer program is used for both; the desired approach is selected with an input key word.

Water Quality Parameters. A total of 26 water quality parameters were specifically identified by EPA for careful attention in this study (and in other Great Lakes studies). The water quality data and the waste load data for the Buffalo River revealed that 57 constituents were deserving of analysis in this heavily-industrialized reach. The simulation model was required to track these many parameters, both conservative and non-conservative. In addition to the conventional treatment of carbonaceous BOD as non-conservative, the model was required to similarly treat nitrogenous BOD, ammonia, organic nitrogen, and phenols. Three distinct deoxygenation rate constants are used in the model.

Reaeration. The industrialized reach of the Buffalo River has extremely low linear velocities. Moreover, the prevailing winds off Lake Erie are persistent and of high velocity. Consequently, the model calculates the reaeration coefficient in two ways: as determined by stream velocity, and as determined by wind velocity. The program selects the larger of the two coefficients for each river segment.

Thermal Analysis. The very large heat loads from industrial sources into the Buffalo River, plus the high residence times for water in this reach and the high wind velocities, required that the model simulate effects upon the river water temperature. The thermal analysis of VERWAQ includes the heat flux from discharges, tributaries, and non-point sources, convection and conduction between the stream and the ambient air, and solar radiation to the stream. Rate constants are then appropriately adjusted for temperature.

Non-Point Waste Loads. The combined sewer overflows (and benthal loads) constitute almost one-third of the total waste loads. The model was required to treat non-point sources as distributed waste loads simultaneously as it treats point sources of other wastes. The Streeter-Phelps equations in differential form were augmented by a distributed waste model (chemical and thermal constituents) and then reintegrated.

In the conventional Streeter-Phelps analysis, the steady-state BOD balance around a differential longitudinal segment of the river (between point-source additions) is composed of three terms: the upstream waste input, the downstream waste output, and the reaction (oxidation) loss in the segment. The analysis for VERWAQ adds a fourth term, the non-point source (distributed) waste input in the distance interval dx: $(QL/R)dx$; where Q, L, and R are respectively the non-point-source total flow rate, the non-point-source BOD concentration, and the longitudinal distance (reach) over which the non-point discharge is evenly distributed.

As in the conventional Streeter-Phelps analysis, the sum of the terms is set equal to zero (for steady-state) and integrated over a longitudinal river distance x. In this analysis, however, the extra non-point-source term is included in the sum and in the integral. The result is solved for the BOD concentration which is then substituted into the equation for deoxygenation rate. Integration of this equation yields the expression for oxygen deficit as a function of longitudinal distance.

Testing of the Model in the Buffalo River

Plug-Flow Model. The plug-flow model was applied extensively to the dredged portion of the Buffalo River, using various values and combinations of values for the constants. Satisfactory simulation of the empirically-determined non-conservative water quality parameters was not achieved, confirming the prior conclusion of significant longitudinal mixing based upon the river hydraulics and upon the empirical water quality data. Typically, the dissolved oxygen profile calculated with the plug-flow model is a decrease in DO from about 7 ppm to near zero in the two-mile reach with the heaviest waste loads. The experimentally-determined dissolved oxygen content, however, was uniformly low (0.0 to 1.8 mg/l) throughout this reach. Despite high values (consistent with high temperatures but still reasonable) for the deoxygenation coefficients, the plug-flow model could not approximate the measured step change in dissolved oxygen content with distance.

Completely-Mixed Model. The completely-mixed modeling option of VERWAQ resulted in excellent agreement (as shown in Table 1) with experimentally-determined data, for conservative parameters and non-conservative parameters (dissolved oxygen, BOD_5, NH_3-N, and phenols), using for the most part constants independently published by others. For all except fluoride and nickel, the calculated values came well within the range of measurements. It is possible that slightly-soluble salts such as fluorides, whose ions originate from different industrial discharges, may exceed their solubilities and precipitate in the river. The model was then adequately verified by comparing its water quality predictions with measured winter time data in a completely different flow rate regime from the upstream tributaries (two to seven times the average summer time flow).

Water Quality Projections

Projected Waste Loads

The projected waste loads into the Buffalo River were based upon implementation of Best Practicable Control Technology Currently Available (BPCTCA). It was projected that three sewage treatment plants currently discharging into Cayuga Creek would be phased out during dry weather as the sewage is incorporated into the Buffalo system. The projected industrial waste loads were based upon existing permits, effluent limitation guideline development documents, interim effluent guidance documents, or Region II permit summary tables; as these were available in October 1973. Several independent judgements were made in the absence, at that time, of promulgated effluent limitations guidelines or of issued permits. It was also judged that several low-volume industrial discharges would be incorporated into the municipal sewer system. It was projected that the combined sewer overflow waste load would remain the same as the present load.

Projected Water Quality and Waste Load Allocations

The developed and verified model was utilized to predict water quality from the projected BPCTCA waste loads. These projected water quality data, for both the average summer time and critical flow conditions, are listed in Table 1. The projected water quality, at critical flow conditions, marginally came within the standards for temperature and dissolved oxygen. However, more stringent waste allocations were recommended for iron. Upon implementation of BPCTCA, which would be effective in reducing most waste loads, the oxygen-demanding waste load of the combined sewer overflows would then become the dominant constraint for achieving good water quality in the Buffalo River.

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Table 1

Water Quality, Dredged Portion of the Buffalo River
Concentrations in mg/l

	Water Quality Criteria (a)	Measured Data				Calculated Present Data (b)	Projected Data	
		No. Data Pts.	Max.	Min.	Average		Avg. Summer Flow (b)	Critical Flow (c)
Dissolved Oxygen	3.0*	76	4.0	0.0	0.94	1.03	3.79	3.06
BOD-5	—	41	14.0	0.6	4.22	4.22	1.89	1.73
NH_3-N	2.0*	29	1.26	0.14	0.69	0.69	0.22	0.21
NO_3-N	4	17	0.59	0.0	0.13	0.42	0.39	0.28
Cyanide	0.1*	28	0.05	0.0	0.01	0.034	0.03	0.038
P-Total	25	28	0.85	0.07	0.29	0.60	0.45	0.55
Sulfate	500	33	68	49	57	60.5	58.6	58.6
Chloride	250	33	70	46	57	51.7	43.2	44.6
Fluoride	1.5	17	0.69	0.44	0.53	1.14	1.09	1.40
Oil & Grease	7	29	7.2	0.1	2.6	3.89	2.23	2.40
Phenols	0.2	29	0.266	0.008	0.027	0.02	0.010	0.013
Arsenic	1.0	12	0.03	0.00	0.02	0.011	0.010	0.014
Barium	5.0	11	0.20	0.0	0.0	0.001	0.0	0.0
Cadmium	0.3*	15	0.00	0.00	0.00	0.004	0.001	0.001
Chromium	0.05	27	0.08	0.00	0.02	0.057	0.015	0.020
Copper	0.2*	24	0.06	0.00	0.02	0.034	0.030	0.037
Iron	0.8	10	5.65	0.68	3.11	3.066	2.054	2.729
Lead	0.1	21	0.23	0.00	0.06	0.071	0.037	0.048
Mercury	0.006	27	0.017	0.000	0.001	0.001	0.000	0.000
Nickel	0.7	12	0.00	0.00	0.00	0.027	0.026	0.036
Selenium	2.5	21	0.004	0.001	0.003	0.000	0.000	0.000
Zinc	0.3*	10	0.178	0.024	0.084	0.098	0.087	0.116

(a) Criteria Labelled * are explicit in N.Y. State Standards
Others are implied by "fish survival" criterion.
(b) Average Summer Flow, Completely-Mixed Model.
(c) Critical Flow, Completely-Mixed Model

STREAM MODELING AND WASTE LOAD ALLOCATION

James Y. Hung, Aolad Hossain and T. P. Chang
Water Pollution Control Division
Indiana State Board of Health
Indianapolis, Indiana

ABSTRACT

The Indiana Stream Pollution Control Board conducted an intensive stream modeling program for Indiana's major rivers during the past three years. These stream models were used primarily for the purpose of waste load allocation. This paper describes the stream self-purification system models for BOD, DO and ammonia. In addition to the analysis of model components, problems of evaluating system parameters are examined. The formulation of the waste load allocation methodology and the issues in allocation implementations are reviewed. The paper is concluded by a discussion of the limitations in using stream models.

INTRODUCTION

The Federal Water Pollution Control Act Amendments of 1972 have established improved river quality as a major goal of overall river basin planning. The tasks of setting water quality standards and determining waste load allocations for dischargers are bestowed upon the State Water Pollution Control Agencies in conjunction with the U. S. Environmental Protection Agency (USEPA). During the past three years, the Indiana Stream Pollution Control Board (ISPCB) has been in the process of building stream quality models for Indiana's rivers.[1] Because dissolved oxygen (DO) is traditionally the main indicator of pollution, a major effort was made to model DO as well as the oxygen consuming parameters such as biochemical oxygen demand (BOD) and nitrogenous oxygen demand (NOD).

In the Indiana Water Quality Management Plan, Indiana streams are divided into ninety-nine segments with forty-two segments classified as water quality limited segments. The criteria of segment classification was based mainly on the projected condition of dissolved oxygen deficiency and the need of advanced waste treatment. Of the ninety-nine segments classified, eighteen segments have been modeled, including the Wabash River,[2] White River,[3] Grand Calumet River,[4] Little Calumet River[5] and the Mississinewa River.[6] The model was designed mainly for waste load allocation purposes and therefore emphasis was placed on a critical condition at low stream flow period.

Objectives of this paper are (1) to describe the rationale, considerations and procedures of ISPCB's stream modeling and waste load allocation processes; and (2) to summarize ISPCB's experience, in particular, the types of problems they encountered during this entire endeavor.

STREAM MODELING

In the selection of model components, it is necessary to consider the local climate and stream conditions as well as the purpose of modeling. Indiana climate is of the humid, continental, warm summer type. It is characterized by definite winter and summer seasons accompanied by wide temperature ranges. Occasionally, stream temperature in the summer months, May to September, can be above 30°C. Annual precipitation averages approximately 38 inches and stream runoff is about 12 inches. Indiana adopts the average seven-consecutive-day, once in ten years low flow in the definition of its water quality criteria. Dry seasons are usually between August and October. Therefore, stream nitrification can be significant during the summer months with low stream flow and high water temperature.

As described earlier, the purpose of modeling is to determine BOD and NOD allocations for municipal and industrial dischargers. Only daily average DO standards were tested against the load allocation, and thus photosynthetic and respiration factors were not considered which cause diurnal DO variations. In view of the fact that the sludge deposit in the stream bed is expected to be reduced due to increasing pollution control measures, benthal demand was also neglected for most segments modeled.

In the ISPCB study, a modified version of the Streeter-Phelps equation for DO deficits was utilized which includes both carbonaceous and nitrogenous biochemical oxygen demands and atmospheric reaeration. The revised Streeter-Phelps equations are as follows:

$$D(t) = -\frac{K_1L_o}{K_2-K_1}\left(e^{-K_2t}-e^{-K_1t}\right) - \frac{K_nN_o}{K_2-K_n}\left(e^{-K_2t}-e^{-K_nt}\right) + D_oe^{-K_2t} \qquad (1)$$

$$L = L_oe^{-K_1t} \qquad (2)$$

$$N = N_oe^{-K_nt} \qquad (3)$$

where:

$D(t)$ = DO deficit at time t.

D_o = Initial DO deficit, mg/l

L_o = Initial carbonaceous BOD, mg/l

L = Carbonaceous BOD at time t, mg/l

N_o = Initial NOD, mg/l

N = NOD at time t, mg/l

K_1 = Carbonaceous deoxygenation rate constant (base e), day $^{-1}$

K_n = Nitrogenous deoxygenation rate constant (base e), day $^{-1}$

K_2 = Reaeration rate constant (base e), day $^{-1}$

The carbonaceous deoxygenation rate, K_1, and the nitrogenous deoxygenation rate, K_n, were determined by the slope of the BOD and NO_3-N profiles respectively when plotted on a semilog paper. The stream reaeration coefficient, K_2, was computed by one of the empirical equations[2] which are functions of stream temperature, stream flow velocity and mean depth. The hydraulic data usually available for flow velocity and depth are taken at the gaging stations. These stations are often located at the control sections of the stream where the flow velocity tends to be higher and mean depth to be smaller than that of the normal stream reaches. Using the above mentioned hydraulic data would tend to produce an overestimated K_2 value. Another source of the hydraulic data is the dye travel study which provides the time of travel information. However, dye studies taken at critical low flow period are very rare. Previous investigators [7,8] have found that general hydraulic equations developed at various ranges of flow can be quite different and that the actual travel time at low flow period is longer than that computed by hydraulic equations for high flows.

When stream DO profile data were available, the model verification was made to compare the computed stream DO profile with the measured profile. In this way, an appropriate equation of K_2 was decided for a particular stream segment. However, complete sets of stream profile data for DO, BOD and NO_3-N are often difficult to obtain. In this case, the choice of a stream reaeration equation would be difficult because various proposed equations[2] could produce quite different results. Frequently, individual judgement must be used in the selection of equations.

Further complications resulted from the fact that our purpose of modeling was waste load allocation. Biochemical characteristics are expected to be different in the effluent and in the stream when additional treatment and additional quantity of wastewater are realized. The deoxygenation rates, both K_1 and K_n, computed from existing measurements can serve only as a reference for predicting future stream deoxygenation rates. The problem of deoxygenation rate prediction is unresolved in the current state of art. Furthermore, there is evidence in our Wabash River study that stream deoxygenation rates are functions of dilution ratio and therefore dependent upon the stream discharge rate, in addition to stream temperature.

The one dimensional modeling of DO, BOD and NOD, such as that represented by equations (1), (2), and (3), may yield poor results in a short reach immediately below the effluent outfall because of the incomplete mixing problem. This is particularly true when the dilution ratio is large. Stream survey data used for ISPCB model verifications were mainly composite samples taken in a twenty-four hour intensive survey. For each stream cross section, samples were taken at center, left side and right side of the stream width. These samples were analyzed separately and their average values were used for model verification.

WASTE LOAD ALLOCATION FORMULATIONS

PL 92-500 requires all dischargers to provide, at the minimum, a secondary wastewater treatment (such as an activated sludge process) for municipal wastewater plants and the best practicable treatment (BPT) for industrial wastewater plants. However, if the predetermined stream water quality standard in the affected segment cannot be achieved as a result of this minimum treatment (defined as a water quality limited segment), then various levels of advanced wastewater treatment (AWT) would be required for some or all dischargers. Methods for determination of each polluter's treatment level (or waste load allocation) in this affected segment then becomes a question for consideration. The problem would be simple if only one discharger was responsible for the affected stream quality. The answer becomes somewhat cloudy when more than one discharger is involved. Proposed solutions to this problem follow two basic approaches[9]: the cost effectiveness approach and the equity approach.

The cost effectiveness approach is a typical mathematical programming problem of the form:

minimize: total treatment costs

subject to: quality standard, physical and technical constraints

Due to the usually nonlinear nature of the cost function associated with the treatment levels, a nonlinear programming solution is generally required.[4] However, the major difficulty in implementing this cost effectiveness approach is the inequality which results from discrimination in treatment requirements. Difficulties may also be encountered when new waste sources enter into this segment and complete readjustments may then be required. In addition, this approach assumes that optimal solution in the stream segment being considered is independent of the influences from both upstream and downstream segments. This, however, is usually untrue.

The second proposed solution is an equity approach in the form:

$$T_1 = T_2 ---- = T_i$$

Subject to: quality goal satisfied, physical and technical constraints

Where T_i = the degree of treatment for the i-th plant. Again, the so-called "degree of treatment" is difficult to define, especially when comparing a privately-owned industrial plant with a publically-owned municipal plant. The present practice in Indiana is to adopt a combination of the two above mentioned approaches. An example is the waste load allocation for the Grand Calumet River Basin.

Academicians have proposed a third but not yet practiced approach,[10] which is to treat the stream assimilative capacity as a commodity and to offer it in a competively open market. The allocations would be settled purely by the balance of supply and demand subject to certain constraint. However, this approach neglects historical factors and would require institutional changes.

Allocation computation in all three approaches requires the predetermination of the relationships between the effluent quality (such as biochemical oxygen demand and ammonia concentration). These relationships can be established through either regressional analysis or simulational analysis (such as the Streeter-Phelps equation for dissolved oxygen). However, the simulational method is generally preferred because it provides better capability in generating alternative solutions such as by-pass piping and timing adjustments.

ALLOCATION RELATED PROBLEMS

Compared to wastewater treatment technology and stream modeling techniques, studies related to wasteload allocation methodology are still in their infancy. No established pattern or criteria exist as to the selection of boundary conditions and loading frequencies in a load allocation computation. For example, the headwater source for a stream segment represents a multiparametric loading which consists of flow rate, temperature and pollutant concentrations such as DO, BOD and ammonia. However, these parameters are not constant but rather stochastic processes. Each parameter follows a given statistical distribution. The problem is one of selecting statistically a reasonable combination of loading concentrations in performing wasteload allocation analysis. The situation becomes more complex when one takes into account simultaneously the stochastic loadings of tributaries as well as treatment plant effluents.

The present ISPCB practice in the selection of boundary conditions and loading frequencies is on a case-by-case basis and the factors considered include dilution ratio, loading characteristics and stream quality criteria for that segment.

The increasing uses of biological treatment processes in treating municipal and industrial wastewater have made it necessary to include stream nitrification in the stream DO analysis, especially where the summer temperature range covers the optimal temperatures of nitrification, that is, between 25°C to 30°C. Under this condition, the conventional concept of a single valued stream assimilative capacity of BOD becomes inadequate because NOD is also involved, and because the carbonaceous deoxygenation rate (K_1) and the nitrogenous deoxygenation rate (K_n) are not necessarily equal. The recent USEPA recommendation to use total oxygen demand, which is defined as the summation of ultimate BOD, NOD and DO, as a single-valued loading allocation would have the same problem. Instead, the analysis would have to provide an optimal combination of allocated BOD, DO and ammonia loadings for an effluent source. The definition of stream assimilative capacity becomes more elusive when multiple point sources scattered over different locations are existent in the same stream segment.

Traditionally, one assumes that critically low DO concentration in the stream occurs at extremely low flow This was not always found to be true in the case of multiple sources distributed at different locations, particularly when presented with both BOD and NOD sag curves. This phenomena occurs because the stream DO profile is formed by the superposition of all individual sag curves. The alternation of the shape and location of each individual DO sag due to the change of stream velocity and temperature can create such an overlapping that the critical DO can take place at a flow rate higher than a seven day, once in ten year stream flow.

IMPLEMENTATION PHASE

Stream modeling and waste load allocation of BOD, NOD and DO are parts of the National Pollutant Discharge Elimination System as well as the State Continuing Planning Process. Once the allocation is determined, it enters into the permit as an effluent limitation. The duration of the permit is usually five years. At the end of the permit duration, ISPCB reevaluates the status of the stream water quality and the program of wastewater treatment technology. It then reevaluates waste load allocations for that stream segment.

A majority of the waste load allocations are presently designed on a year round basis. In some cases, separate allocation values are given for summer months and for winter months. Eventually, the waste allocation may require a detailed operational schedule for effluent limits on a monthly basis or directly tied to daily climate and stream flow conditions. This process would require a higher degree of scientific sophistication and management which could become an overwhelming administrative task under the present understaffed condition in the ISPCB.

DISCUSSION AND SUMMARY

Computer modeling of stream self-purification systems is a useful tool for water quality management, especially in a dynamic program like waste load allocation. However, when applying this tool one has to be mindful of its limitations and a certain degree of flexibility and precaution are required. First, not all aspects of stream self-purification systems are understood at the present stage of development. The first order differential equation currently used for describing the self-purification systems has its shortcomings, notably in dealing with stream nitrification, which is a two-stage process. Furthermore, the K rates in the Streeter-Phelps equation are not constants and their predictabilities are uncertain. As a result, model verification can be difficult. Secondly, complete sets of climate and stream quality information are often not available in the calibration of model characteristics and individual judgement has to be substituted. Thirdly, due to the incompleteness of the allocation criteria relative to boundary and loading frequencies, case-by-case negotiations and compromises based on local circumstances are unavoidable in load allocation determinations.

Although the problems discussed in this paper are for BOD, NOD and DO, similar problems also exist for thermal and conservative pollutants. The situation could become even more complex if effects of nonpoint source pollutants are taken into consideration.

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AFFILIATIONS OF AUTHORS

Drs. James Y. Hung, Aolad Hossain and T. P. Chang are presently serving as Acting Chiefs of the Engineering System Section, the Computer Modeling Section and the Program Support Branch, respectively, Water Pollution Control Division, Indiana State Board of Health, Indianapolis, Indiana.

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PATUXENT RIVER BASIN MODEL
RATES STUDY

Thomas H. Pheiffer
Leo J. Clark
U. S. Environmental Protection Agency
Region III
Annapolis Field Office
Annapolis, Maryland

Norman L. Lovelace
Water Division
Water Planning & Standards Branch
U. S. Environmental Protection Agency
Region IX
San Francisco, California

ABSTRACT

During the summer seasons of 1973 and 1975, intensive water quality surveys were carried out in the Patuxent River Basin for the purposes of mathematical model calibration and validation. In the summer of 1973, the Patuxent was receiving secondary effluent from eight major municipal treatment plants. No significant industrial waste discharges are present in the Patuxent system. A steady state water quality model was calibrated and validated using the data collected from the 1973 field surveys. During 1975, a major treatment plant was upgraded to include high BOD removal and nitrification; new field surveys were conducted and the model was recalibrated and validated to reflect changes in the instream reaction rates* as a result of the changed effluent characteristics. This paper discusses the field studies, data results, model application procedures and perhaps most importantly, how the procedures that were used could be improved.

BACKGROUND

The state-of-the-art of modelling is such that mathematical expressions can be written and translated into computer programs to represent complex environmental interactions. However, too little effort is being directed towards defining the numerous variables and/or biological coefficients required to make these mathematical expressions either descriptive or predictive. Much effort is being devoted to studying the mathematical behavior of these equations and expressions, but not enough is being given to real world applications.

A basic, but essential problem confronting many modellers is what instream reaction rates to assume for carbonaceous decay and nitrification when treatment is upgraded above the conditions that existed when field data was collected. To date, estimates of reaction rates for highly treated municipal effluents are based solely on the best judgement of modelling experts, not on well documented field data. With this in mind, the Annapolis Field Office (AFO), Region III, EPA, has attempted to define changes in instream reaction rates resulting from the upgrading of a major wastewater treatment plant, in particular, the Parkway Plant of the Washington Suburban Sanitary Commission, located near Laurel, Maryland.

STUDY AREA

The Patuxent River, located entirely within the State of Maryland, has a drainage area of approximately 930 square miles. Its two major tributaries are the Little Patuxent River and the Western Branch with drainage areas of 160 and 110 miles, respectively. The tidal portion extends to Hardesty, Maryland, a distance of 54 miles from the mouth of the estuary.

The headwaters of the Patuxent are impounded above Laurel, Maryland in the Triadelphia Reservoir and the T. Howard Duckett Reservoir (Rocky Gorge). The Rocky Gorge Dam provides for a generally regulated flow in the mainstream of the Patuxent downstream to the confluence of the Little Patuxent with the mainstem, a distance of 17.5 river miles. During the summer months, this regulated flow amounts to approximately 10 million gallons per day (mgd) or 15 cubic feet per second (cfs). It is in this critical reach (17.5 miles) that stream quality was improved by upgrading the Parkway Wastewater Treatment Plant.

The Little Patuxent is not regulated by dams and exhibits irregular flow patterns following thunderstorm activity. Surging flows into the estuary during the summer are attributed mainly to the Little Patuxent. Total annual precipitation in the basin is estimated at 30-44 inches per year with the maximum precipitation occurring in July or August.

DESCRIPTION OF STUDY

For the purpose of obtaining data for model application, 52 water quality sampling stations were located in the Patuxent River Basin. Twenty-seven of these stations were located in the estuary between river mile 0.0 and 54.0. Fourteen stations were located in the free flowing mainstream of the Patuxent between river mile 54.0 and river mile 81.0 at Laurel, Maryland downstream from Rocky Gorge Dam. Eleven sampling stations were established in the Little Patuxent from its confluence with the mainstem upstream to Savage, Maryland, river mile 18.0.

Water quality surveys were carried out in the Basin during April 3-5, June 4-7, July 9-12, and October 9-12, 1973. The June and July intensive surveys encompassed the entire Basin. The April and October surveys were confined to the estuary with the April survey designed to determine rough salinity gradients for estimating dispersion coefficients. The October survey measured surface and bottom dissolved oxygen concentrations for model verification. Data collected in the estuary were obtained during slack water conditions.

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* Reaction rates refer to first order rate constants. The models used in these studies use first order rate expressions to represent the nitrification and carbonaceous deoxygenation processes. The question of whether a first order representation of these processes is the most realistic is not a point of discussion for this paper.

During the period of July 28-31, 1975, an intensive water quality survey was carried out in the critical reach of the free-flowing Patuxent from below the dam of the Rocky Gorge Reservoir (mile 81) downstream to the head of tide (mile 54). The purpose of this survey was to obtain data for recalibration of the existing model. The Parkway Plant located at river mile 74.5 had gone on line during January, 1975 with advance waste treatment (AWT). Next, a survey was initiated from October 14-16, 1975, to obtain data to validate the reaction rates determined from the July 28-31, 1975 survey data.

Flows for the studies were obtained from stream discharge gages located in the free-flowing portion of the Basin. The United States Geological Survey made current meter discharge measurements at each site during the June and July, 1973 studies and again prior to the 1975 surveys. This enabled the USGS to furnish stream discharges for the gage heights read at the time of sampling. The samples were analyzed at the Annapolis Field Office laboratory during the 1973 and 1975 surveys for the following parameters: DO, BOD_5, TOC, TC, TKN, NH_3, NO_2+NO_3, Pi, TP and Chloro a. Salinity, conductivity, temperature and pH were routinely measured in the field.

Special studies during 1973 included long-term BOD measurements at specified estuarine and stream stations for the purpose of attempting to measure in-stream carbonaceous and nitrogenous oxygen demand rate constants. Methyl blue, an inhibitant to the bacterial oxidation of ammonia nitrogen, was injected into duplicate samples to determine the second stage oxygen demand (nitrogenous BOD). Again, during July 28-31, 1975, in the critical reach below the Parkway AWT Plant, an attempt was made to follow a specific parcel of water based on time-of-travel data obtained during the week of June 30, 1975. Long-term BOD and the nitrogen series were run on samples from the selected stations below the discharge of the Parkway AWT Plant.

Twenty-four hour composite samples of wastewater treatment plant effluents were obtained from the major plants in the basin during the June and July, 1975 surveys. Composite treatment plant data were also available from a survey by the Annapolis Field Office during October, 1972. The nine plants shown in Figure 1 account for approximately 96% of the treated wastewater discharged in the entire basin. During the 1975 surveys, only the wastewater treatment plants in the critical reach of the mainstem of the Patuxent were sampled. These included the Maryland City, Parkway and Bowie-Belair Plants.

DATA ANALYSIS

This discussion and those that follow will focus on the critical reach of the free flowing Patuxent, i.e., from below the Rocky Gorge Dam (mile 81) downstream to the head of tide (mile 54). As previously mentioned, the Parkway Plant is located at river mile 74.5 in this segment.

The data comparisons discussed below will concern the water quality data collected during the July 9-12, 1973 and July 28-31, 1975 surveys. The low flow conditions were essentially the same, 36 cfs in 1973 and 31 cfs in 1975, at the Baltimore-Washington Parkway (mile 75) just above the Parkway Plant. Likewise, stream temperatures were similar in the segment, i.e., 23°C in 1973 and 24°C in 1975.

FIGURE 1

PATUXENT RIVER BASIN

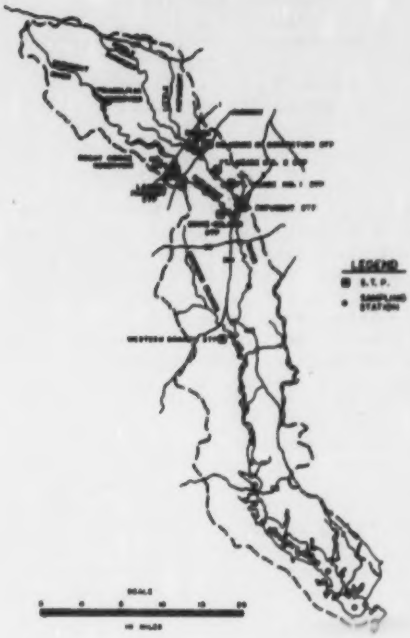

Figure 2 illustrates the improvement in D.O. levels between the 1973 and 1975 July surveys. The average D.O. concentration at mile 71.5 for the 4 day survey periods increased from 5.1 mg/l (7/9-7/12, 1973) to approximately 5.9 mg/l (7/28-7/31, 1975). The minimum observed concentration increased from 3.1 mg/l to 5.5 mg/l for the same periods.

At this point, it is important to note the recent modifications to the Parkway Plant. Its design flow has been expanded from a 2.4 mgd secondary facility to a 7.5 mgd AWT plant. The AWT plant went on line during January, 1975. The current monthly average flow through the plant is 4.5 mgd. It should be noted that the secondary facility was overloaded during the 1973 studies. In 1973, the flow was about the same as the current 4.5 mgd.

Prior to expansion, the Parkway Plant was a secondary facility utilizing trickling filters. The expanded plant encompasses the trickling filters plus an activated sludge system which achieves high BOD removal and the nitrification of ammonia nitrogen to nitrate nitrogen. Microstrainers have been added to further reduce the suspended solids. The effluent then goes through a chlorine contact chamber and is aerated prior to discharge to the Patuxent (1). This added aeration process has resulted in D.O. levels of 7-8 mg/l in the AWT effluent. In July, 1973, D.O. effluent

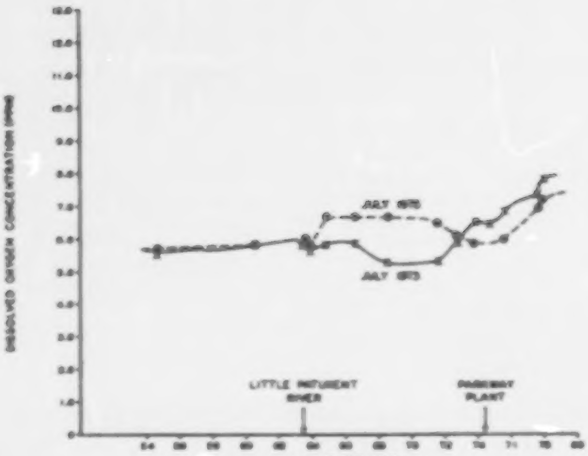

FIGURE 2

levels were 4-5 mg/l in the absence of aeration and with secondary treatment.

During July, 1973, the typical wastewater reductions achieved at the Parkway Plant amounted to 83% for BOD_5 and 17 mg/l for TKN. The ammonia levels comprised about 90% of the TKN in the July, 1973 effluent. The AWT effluent during July, 1975 showed good levels of BOD removal, averaging 5.5 mg/l BOD_5, while TKN averaged 7.1 mg/l, the removal rate being 98% for BOD_5 and 72% for TKN. During August, 1975, the plant achieved an 85.8% removal of TKN. A 95% BOD_5 reduction is the norm at the Parkway AWT Plant.

With the above background information in mind, one would naturally expect accompanying reductions in BOD and TKN downstream from the Parkway Plant. The average ammonia levels for the July 9-12, 1973 and the July 28-31, 1975 periods decreased from 2.7 to 0.5 mg/l at river mile 73.7, a mile below the plant, and from 0.5 to 0.09 mg/l at mile 66.4, about 8 miles below the Parkway discharge and just above the Bowie-Belair discharge. The NO_2+NO_3 levels at the same two stations for the two periods increased from 1.3 to 3.5 mg/l and from 1.4 to 3.0 mg/l for 1973 and 1975, respectively. The NO_2+NO_3 1973 data indicate no instream nitrification of NH_3 to NO_2+NO_3, even though there was evidence that nitrification was occurring (see NH_3 results above). The large increase in NO_2+NO_3 during July, 1975 was due to the Parkway Plant effluent containing around 10-12 mg/l NO_2+NO_3. The apparent loss of nitrogen from the system will be addressed later in this paper. Also, there were corresponding reductions in instream BOD_5 concentrations. For example, the July, 1973 BOD_5 averaged 5.0 mg/l below the plant (mile 73.7) and 3.0 mg/l at the end of the reach (mile 66.4). July, 1975 data showed a general average of 1.0 mg/l BOD_5 throughout the reach.

MODEL APPLICATION

Two models from the CMS (Comprehensive Modelling System), a system of mathematical models developed by Crim and Lovelace, were applied to the Patuxent River System. The two models used were AUTOSS and AUTOQD (2).

Both AUTOSS and AUTOQD contain a hydraulic component, that computes the streamflow profile, and a water quality component that computes concentration profiles. The models are one-dimensional, single channelled models that use first order kinetics to represent instream bio-chemical processes. AUTOSS is a steady state model while AUTOQD is a quasi-dynamic model. AUTOQD represents flow patterns as step-shaped patterns in time, and water quality concentrations as continuous patterns.

Data on the free flowing portion (for the period July 15-19, 1968) were available from a cooperative study with the Maryland Department of Water Resources. Both the 1968 and the 1973 data show the mainstem to contain high concentrations of TKN nitrogen. These high nitrogen concentrations were attributed to wastewater treatment plant discharges of excessive amount of TKN and NH_3 forms of nitrogen.

AUTOSS was calibrated to simulate DO conditions in the mainstem for the periods July 15-19, 1968 and June 4-7, 1973. Ultimate carbonaceous (CBOD) and nitrogenous (NBOD) BOD loadings from the treatment paints were entered into the model at the appropriate river miles. The ultimate CBOD and NBOD loadings were calculated from the commonly used literature values where ultimate CBOD = 1.45 BOD_5* and ultimate NBOD = 4.57 TKN. Relatively steady state low flow conditions occurred during July, 1968 and medium flow conditions occurred during June, 1973. The out flow at the downstream junction of the model was 120.1 cubic feet per second (cfs) and 458.3 cfs, respectively. Stream velocities used in model calibration were obtained from 1968 and 1975 studies by the Annapolis Field Office of time-of-travel and from depth measurements made during 1973 studies.

During the period of July 9-12, 1973, an average net flow of 152.3 cfs was recorded in the mainstem of the Patuxent. The calibrated coefficients obtained from the July, 1968 and June, 1973 model runs were used in the model validation runs. Treatment plant discharge values for carbonaceous and nitrogenous oxygen demand loadings used in the model reflected the results of the composite sampling of July 10-11, 1973. Observed DO values were assigned to major inflows while a DO of 5.0 mg/l* was used for treament plant effluents. The model verification curve for this flow period and the June 4-7, 1973 calibration are shown in Figure 3. Documentation of the 1973 studies including model application to the estuary is set forth in Technical Report 58, by Pheiffer and Lovelace (3).

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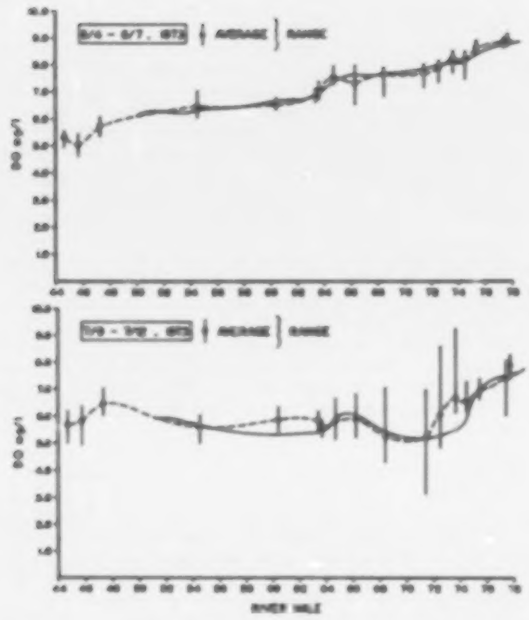
* D.O. data were not taken for the final effluent just prior to its discharge to the stream. This was an unfortunate oversight since effluents comprise a substantial portion of the total flow in the Patuxent above confluence with the Little Patuxent.

FIGURE 3



MODEL RECALIBRATION

As stated earlier, the Parkway AWT Plant went on line in January, 1975. This necessitated adjustments to the existing model which had been calibrated and verified on instream reaction to the discharge of secondary treated effluent from the Maryland City (mile 77.5), Parkway (mile 74.5), and the Bowie-Belair Plants (mile 64.5). With this knowledge, the July 28-31, 1975 intensive survey was planned to encompass the critical reach from below Rocky Gorge Dam (mile 81) downstream to the head of tide (mile 54). The Washington Suburban Sanitary Commission maintained a low flow similar to the July 9-12, 1973 flow condition, at the Rocky Gorge Reservoir for the study period. Instream temperatures resembled July, 1973 water temperatures.

Utilizing the July, 1973 and the July, 1975 stream data, two independent methods were employed to determine reaction rates for the carbonaceous biochemical oxygen demand (CBOD) and the nitrogenous biochemical oxygen demand (NBOD). First, a semilogarithmic graphic solution of plotting stream station loadings (lbs/day) versus travel time in days was used. Next, the reaction rates obtained from the semi-log plots were tested in the model. Only through model testing of the rates and a knowledge of the stream can the modeller select the best values which work in the model and yet do not compromise the field data.

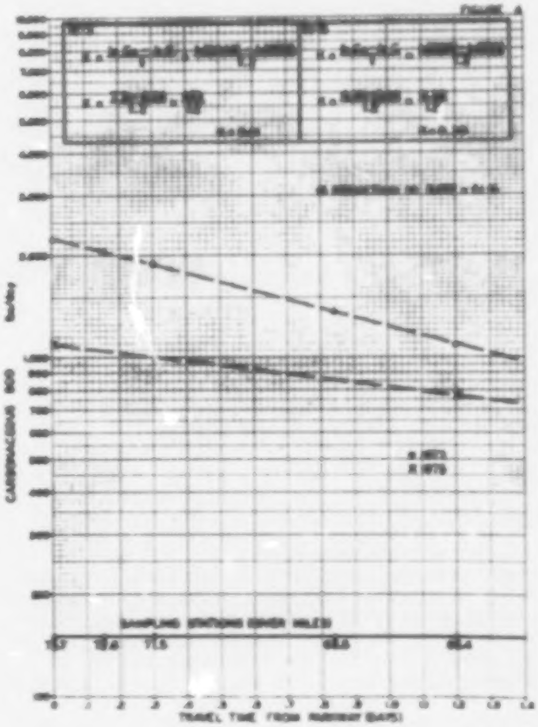
The above methods for rate determination were employed for the calibration of the 1973 version of the model, i.e., the one validated when the critical stream segment was receiving secondary effluent only. The existing version of the model was recalibrated from rate determinations based on the July 28-31, 1975 stream data. This calibration reflects the effect of the Parkway AWT Plant discharge from mile 74.5 downstream to mile 64.5.

CONCLUSIONS

Figures 4 and 5 are semi-log plots of the July, 1973 and July, 1975 CBOD and NBOD loadings at stream sampling stations in the critical reach below the Parkway Plant, mile 73.7 to 66.4. These plots are intended to graphically show the reduced loadings for both CBOD and NBOD due to improved treatment at the Parkway Plant. As previously discussed, the stream flow conditions and stream temperatures are nearly identical for the two study periods.

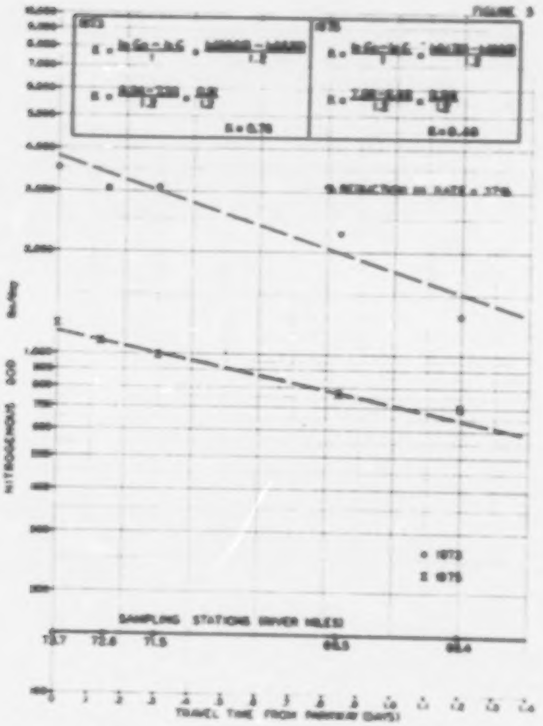
Figure 4 shows a reduction in the CBOD decay rate of 51% due to higher BOD_5 removal at the Parkway Plant. The K rates determined were 0.61 (1/day base e) for the period July 9-12, 1973 and 0.30 (1/day base e) during July 28-31, 1975. It should be noted that only two reliable data points, mile 73.7 and 66.4, were obtained from the long term BOD studies. The grab samples were not dechlorinated as were the long term samples, thereby giving low, erratic BOD_5 values.

FIGURE 4



The conclusion drawn from Figure 5 is that the K rate for NBOD has been reduced 37% with the addition of nitrification at the Parkway Plant. The determined K rates for NBOD decreased from 0.76 (1/day base e) in 1973 to 0.48 in 1975.

FIGURE 5



The rate that best fit the 1973 version of the model for the decay of CBOD was 0.62 (1/day base e) in the critical reach below the Parkway Plant. The CBOD rate tested in the 1975 model was 0.40 (1/day base e). Even with the restriction of limited BOD data for the July, 1975 period, the rates used in the model pretty much paralleled those determined graphically.

For NBOD, a K rate of 0.65 was used in the upper half of the critical reach in the 1973 model, while a rate of 0.45 worked best in the lower end of the reach. The calibrated rates for the 1975 model were 0.50 and 0.27 in the same segments.

Figure 6 represents a sensitivity analysis of the model decay rates discussed above. Three separate model runs were made. First, the 1973 rates were used to predict the July, 1975 DO field data. These rates gave a better fit in the lower half of the critical reach, but not at the sag point. Next, the 1975 graphic rates were plugged into the model. Thirdly, the graphic rates were increased for NBOD decay in an attempt to get the best calibration. However, no rates were adjusted to the point where the TKN and BOD field data were compromised. As indicated by Figure 6, the model prediction with the calibrated rates predicted higher DO levels in the lower part of the critical reach. The discussion section which follows, will address the need for further field studies and model adjustments. However, the calibrated decay rates were tested with an independent set of data for October 15-16, 1975, and the model predicted DO quite accurately in the sag area at the discharge point of the Parkway AWT Plant.

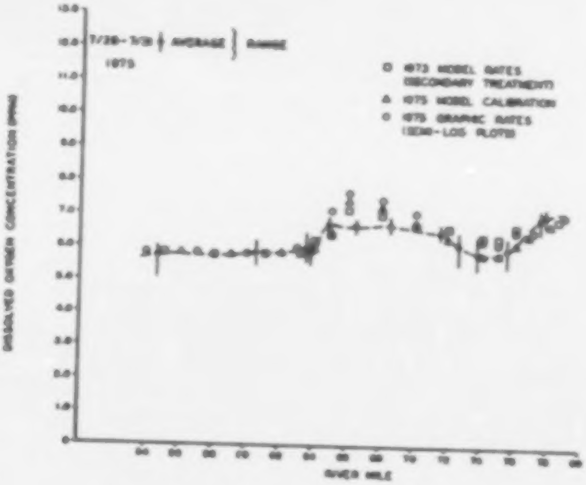


FIGURE 6

The general conclusion to be drawn in this paper is that modifications to model rates due to changes in stream loadings, changes in discharge locations, etc., should be based on estimates from actual field data. The best way to estimate these decay rates for free flowing streams is not by curve fitting with the existing model. Rather, free flowing stream rates should be obtained by plotting semi-logarithmically the actual stream segment loadings versus travel time. These rates can then be adjusted to calibrate the model (but not to the degree that the BOD and nitrogen data are compromised) so that DO prediction profile matches the field data.

DISCUSSION

The investigators realize that there are shortcomings in the studies both in terms of data requirements and model simulation. The contribution of this paper to the state-of-the-art review of modelling might best be described as the basic awareness of the investigators of the need to update a model when the conditions on which that model had previously been validated have changed and the realization that field studies must be carried out to define changes in model coefficients due to modifications in wastewater inputs to the model.

Additional studies seem warranted to further define instream changes in the decay of CBOD and NBOD below the Parkway AWT Plant. Field studies should again be carried out during a steady state, low flow condition accompanied by warm weather stream temperatures. The nature of effluents from the Maryland City, Parkway and the Bowie-Belair Plants must be better defined. The results of 24 hour composite samples might not truly represent the proper numbers for BOD and nitrogen to use as a steady state input. Either hourly grab samples or a daily grab sample at discrete plant flow periods should be obtained. A weighted average of these samples results could give more reliable numbers for model usage. In addition, a firm fix on the DO level of the final plant(s) effluent should be established for a typical warm weather condition.

Future studies should delineate the effluent plume in order to determine the extent of instream mixing, the rate of decay by the microbial population within the plume area, and the configuration of the plume so that the stream sampling below the point of discharge can be designed to represent a composite analysis of stream quality in that segment. In addition, oxygen sediment demand should be measured at and below the point of discharge in an attempt to quantify the affects of any sludge deposits on the oxygen content of the overlying water. Benthic oxygen demand should be quantified throughout the entire critical segment in order to substantiate any assumption made regarding background oxygen demand or depletion.

The investigators strongly feel that more visual observations are needed in the critical area where they are trying to define instream reaction rates. As noted earlier, the data for 1973 indicate that nitrification of NH_3 to NO_3 appears to occur. However, the reduction of NH_3 does not result in a corresponding increase in NO_3. Rather, the data indicates a loss of nitrogen from the system. The loss of nitrogen through instream denitrification does not appear probable, since DO levels do not approach anoxic conditions. Algae cannot account for this decrease, since chlorophyll a levels are and have been extremely low, i.e., 1-10 μg/l in the free flowing Patuxent. Rooted aquatic plants, or other shoreline vegetation, if present in sufficient quantities, could account for the nitrogen loss from the water column by plant utilization of the inorganic forms of nitrogen as well as affecting the DO budget on a diurnal basis. This possibility should definitely be investigated, since field biologists with the State of Maryland have indicated the presence of rooted aquatic plants in the study area.

It is recognized that BOD is not the ideal parameter for determining rates. One reason is that laboratory error is often high. In the Patuxent, chlorine in the stream samples gave erroneous values in some instances, though once the chlorine was detected, it was destroyed in the laboratory before BOD was run. But, if BOD is to be used for rate determinations, sufficient BOD measurements should be taken to make the rate determination statistically valid.

It should be noted that the models discussed in this paper were used by the State of Maryland in 1973 to evaluate effluent limitations proposed for wastewater treatment plants in the Patuxent River Basin Water Quality Management Plan (4). The recalibrated model (1975) of the free flowing mainstem was also given to Maryland at the request of the Maryland Water Resources Administration.

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EFFICIENT STORAGE OF URBAN STORM WATER RUNOFF

J. Robert Doyle
US Environmental Protection Agency
Denver, Colorado 80201

James P. Heaney, Wayne C. Huber and Sheikh M. Hasan
Department of Environmental Engineering Sciences
University of Florida
Gainesville, Florida 32611

Summary

A mixed integer linear programming model is used to evaluate alternatives for use of storm water detention in flood plains and developing areas. This model is suitable where a refined analysis is needed. Mixed integer programming is appropriate when it is necessary to handle fixed charge problems. This added feature significantly increases the computational complexity of the model as compared to standard linear programming procedures. Given an inventory of available storage sites, both in and out of the flood plain, and costs for other flow reduction measures, the optimization model determines the least costly combination of storage reservoirs. Application to the Hogtown Creek drainage basin in Gainesville, Florida is included to demonstrate the techniques.

Introduction

Storage facilities for controlling the quantity and quality of urban runoff are becoming increasingly popular.[1] Urban areas have numerous storage options available such as natural depressions, rooftops and parking lots within the drainage basin in addition to storage in the flood plain itself. The model presented in this paper addresses one part of the analysis regarding selecting the number and capacity of reservoir sites. The objective is to find the least costly way of providing a specified level of service. Other considerations regarding environmental impacts, implementation problems, etc., are not considered here. Hasan presents procedures for examining these other considerations.[2]

The Decision Model

A mixed integer programming model was used to evaluate alternatives for storing urban runoff.[3] The objective is to minimize the cost of storing water for a specified level of runoff control. The model provides the engineer or urban planner with a method for evaluating the complete drainage system and utilizes simplified information from each subsystem to test the consequences of instituting various land use or water management plans.

The objectives of the runoff control model are:

1. to synthesize hydrologic, land use, and runoff control cost data from all parts of an urban watershed in order to evaluate a storm water runoff alternative;
2. to find the least cost solution to the problem of maintaining natural stream flows within an urbanizing watershed, thus deriving certain water quality benefits; and/or
3. to assign the responsibility for control of urban storm water quality to land developers and owners by specifying an allowable rate of runoff from their lands.

The complete mixed integer programming model is listed below with each equation or function discussed subsequently.

$$\text{Minimize } Z = \sum_i (S_i u_i + \lambda_i D_i) + \sum_k [(T_k v_k) + \sum_l (\phi_{kl} C_{kl})] \qquad (1)$$

subject to

$$\sum_j X_{ij} + S_i - \sum_m X_{mi} - R_i = 0 \quad \text{for all } i \qquad (2)$$

$$T_k + R_k = P_k \quad \text{for all } k \qquad (3)$$

$$S_i - S_i \lambda_i \leq 0 \quad \text{for all } i \qquad (4)$$

$$R_k - \sum_l (P_k - t_{kl}) \phi_{kl} \geq 0 \quad \text{for all } k \qquad (5)$$

$$\sum_l \phi_{kl} = 1.0 \quad \text{for all } k \qquad (6)$$

where Z = the total fixed and variable cost of storm water storage in the flood plain and all sub-basins,

i = number designating a node; flood plain storage site or stream junction,

S_i = units of water stored at flood plain site i,

$\bar{S}_i$ = total capacity of storage site i,

u_i = unit cost of water stored at site i,

λ_i = 1 if storage site i is used, 0 otherwise,

D_i = fixed cost of site i,

k = number designating a sub-basin,

l = number designating a sub-basin storage alternative or alternative combination in sub-basin k,

T_k = volume of water stored in sub-basin k,

v_k = unit cost of water stored in sub-basin k,

ϕ_{kl} = 1 if sub-basin storage alternative l in sub-basin k is used, 0 otherwise,

C_{kl} = fixed cost of storage alternative l in sub-basin k,

X_{ij} = volume of water which flows from node i to downstream node j,

X_{mi} = volume of water which flows from upstream node m into node i,

R_i = volume of water entering flood plain site i ($R_i = R_k$),

R_k = volume of water leaving sub-basin k,

P_k = volume of runoff entering sub-basin k, and

t_{kl} = storage capacity of alternative l in sub-basin k.

The objective function, equation (1), is minimized in order to obtain the least total cost, subject to certain constraints. The first summation in the objective function is the total variable cost, $(S_i u_i)$, and fixed cost, $(\lambda_i D_i)$, of flood plain storage throughout the watershed. The second summation in the objective function is the total cost associated with use of all sub-basin storage alternatives, the first term being the variable cost, $(T_k v_k)$, and the second term being the fixed cost $(\phi_{kl} C_{kl})$.

Determination of the least cost is subject to the physical laws of continuity. Continuity constraints are written for stream flows in the flood plain and flows within each sub-basin as shown by equations (2) and (3), respectively. Continuity of stream flow must be maintained at every point or node in the network where two or more streams join or where storage is permitted. These constraints specify that the difference between the water volume which flows into and out at a given point must be stored at that point. Therefore, equation (2) requires that storage at node i, (S_i), equals the difference between the storm water inflow, $(\sum_m X_{mi} + R_i)$, and downstream releases, $(\sum_j X_{ij})$. Equation (3) states simply that within sub-basin k, storage plus releases to the flood plain, $(T_k + R_k)$, must equal the total runoff volume entering the sub-basin, (P_k).

The variables λ and ϕ of the objective function can only take on values of either 0.0 or 1.0. When one of these variables is set equal to 1.0, a fixed charge is incurred; when the value is 0.0, no charge is incurred. Each of these zero-one variables is associated with a possible storage site, such that if any amount of water is stored there, the zero-one variable should be set to 1.0. In fact, when solving for the optimal continuous solution, it is very possible that many of the zero-one variables will be set at values between 0.0 and 1.0. If this is the case, a branch and bound procedure is used to determine the optimal mixed integer solution in which all zero-one variables take on integer values. The functional inequalities (4) and (5) are zero-one inducement constraints.

The first of these zero-one constraints, inequality (4), is related to flood plain storage sites and performs two functions in the decision model. The first function is to force at least a portion of the fixed cost to be incurred at a used storage site when solving the problem for the optimal continuous solution. This is necessary to ensure the proper behavior of the model. The second function is to increase the efficiency of the branch and bound procedure in finding the optimal mixed integer solution. For all flood plain storage sites, the storage volume used, (S_i), must be less than equal to the site's storage capacity, $(\overline{S}_i)$.

The second zero-one inducement constraint set, inequality (5), is required for sub-basins which have fixed cost storage alternatives. These storage alternatives are actually combinations of potential storage sites which might be utilized within a single sub-basin. Therefore, these alternatives are mutually exclusive. Equation (6) specifies this mutually exclusive condition by requiring that the sum of all ϕ terms (one term associated with each alternative) within a sub-basin equal 1.0. The branch and bound integer solution procedure will require that the ϕ terms equal either 0.0 or 1.0. Therefore, inequality (5) actually specifies the relationship between the variables R_k and ϕ_{kl}. For a given value of R_k, the ϕ_{kl} term associated with the alternative with the lowest fixed cost and sufficient storage capacity, (t_{kl}), to satisfy the continuity conditions specified by equation (3), will be set equal to 1.0. Within sub-basin k, all other ϕ terms will be set equal to 0.0.

All variables of the decision model must take on nonnegative values. The variables which represent stream flow volumes and storage volumes also have a specified upper bound. The stream flow variables have an upper bound, $(\overline{X}_{ij})$, equal to the estimated natural stream flow volume over a set time period. This upper bound is calculated through simulation of the natural hydrograph representing conditions prior to urbanization, thus constraining urban storm water runoff to rates which existed under natural conditions. The upper bound on storage volume for each facility is set by the feasible limitations of storing water in each facility.

The mixed integer programming model was run using the IBM MPSX package. It is relatively expensive to utilize and is not widely available. If the fixed charge part of the problem is eliminated, then one can use standard linear programming codes which are widely available. Thus, this approach is appropriate for more refined investigations.

The Study Area

Hogtown Creek is the major natural drainage system for the western portion of Gainesville, Florida, where the University of Florida is located. The drainage basin has an area of around 13,000 acres and is made of two predominately different land forms. The southern part of the basin is primarily low lands in which water collected throughout the watershed is eventually recharged to the ground water system.

In contrast, the northern part of the basin comprises uplands which have been extensively developed in some areas with more outlying areas currently undergoing suburban development. However, a significant amount of natural and agricultural land still exists.

Increasingly severe downstream flooding problems associated with upstream development led to the passage of a flood plain ordinance which included provisions to retain runoff peak flows and volumes at their predevelopment levels. As a result of this ordinance numerous detention facilities are in operation in the basin. This modeling application was made to provide some guidance in comparing the suitability of alternative sites.

The decision model is set up by partitioning the entire drainage basin into the twenty subcatchments shown in network form in Figure 1. The appropriate continuity equations are written according to this network utilizing the general form shown by equations (2) and (3). Constraints established by estimating natural hydrologic conditions and storage capacities are used in equation (3), and inequalities (4) and (5).

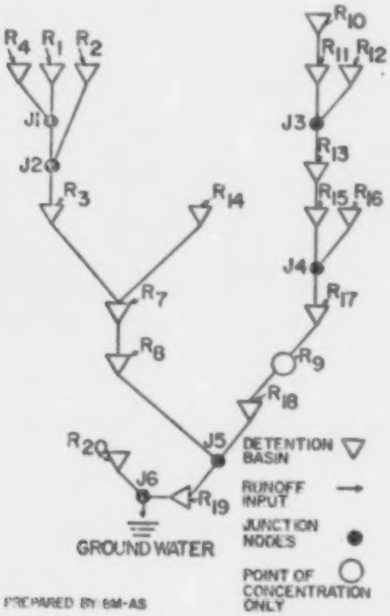

Figure 1. Hogtown Creek Network Flow Diagram

Variables for which input values must be determined prior to running the model are discussed below.

Fixed and Variable Costs, D_i, C_{kl}, u_i, v_k

The fixed cost of flood plain storage at site i, D_i, and of storage alternative l in sub-basin k, C_{kl}, were assumed to be $1,500 per acre of land. The unit costs of water stored at site i, u_i, or in sub-basin k, v_k, were assumed to be $350 per 1,000 ft^3.

Runoff Volume, P_k

Soils information, along with assumptions about the natural vegetative and hydrologic conditions of the watershed, were used to calculate natural stream flow hydrographs.[4] [5] All hydrographs were calculated utilizing a design event with a recurrence interval of 3 years and a rainfall intensity of 0.31 inches per hour for a duration of 15 hours. These hydrographs were used to establish stream flow constraints for use in the decision model and were calculated using a computer simulation model which required runoff coefficients and times of concentration as inputs.[6]

In order to examine ultimate urban conditions, the study area was first categorized into developed and undeveloped areas. The developed area was further broken down into land use types to determine runoff coefficients.[7] The undeveloped area was categorized by projected land use, which was predominantly residential.[8] The same runoff coefficients used for existing land use categories were used for future land uses, with the exception of residential use. In areas where soils were known to have good drainage characteristics, the use of grass-lined swales in residential areas was assumed. Runoff coefficients were calculated for the projected residential areas by taking into account the use of grass-lined swales for drainage. For each hydrograph the volume of water which flowed from the respective sub-basins during a 75 hour time period, assuming no sub-basin storage, was used as the input variable, (P_k), the total runoff volume into sub-basin k.

Capacity of Storage Sites, $\bar{S}_i$ and t_{kl} and Streamflow Volumes, $\bar{X}_{ij}$

The study area was surveyed to determine potential storage sites for storage within the flood plain, ($\bar{S}_i$), and to estimate each site's storage capacity and land area. Within each sub-basin, significant available sites, e.g., wetlands, were inventoried to determine t_{kl}. Sub-basin storage capacity was limited to the runoff entering the sub-basin. An upper limit on stream flow volume, ($\bar{X}_{ij}$), was determined based on maintaining bank stability.

Results

In solving the problem, the model allocates the specified total potential runoff volumes from each sub-basin among the sub-basin and flood plain storage sites, while allowing only a specified volume of runoff to flow downstream. The model results for this example are shown in Tables 1 and 2.

Table 1 shows how the flow volumes were allocated to flood plain storage sites while maintaining as a maximum flow volume the natural stream flow conditions. In order to minimize storage costs, the flow volumes are set near to the natural flow conditions. However, only for a few stream reaches are the flow volumes equal to the maximum limit. These stream reaches form a constraint for upstream flows. Two reaches show a zero flow which should be changed by specifying a minimum allowable flow volume different than zero. Depending on the minimum volumes specified for each reach, this added constraint could significantly alter the results given for this example.

As shown in Table 1, almost all of the flood plain storage sites were utilized to capacity. The cost of utilizing these sites was calculated from the land area required for each site if filled to capacity. The cost-effectiveness of the various sites is not the same because the capacity/area relationship (and therefore capacity/cost relationship) differed for each site. However, almost all sites were fully utilized because the cost of flood plain storage was generally much less than storage within the sub-basins.

Table 2 summarizes all storage allocations and costs. Only in sub-basin 7 was the total storage capacity utilized. This is because this sub-basin contained the natural depression sites which were estimated to cost much less than constructing storage facilities. In all other sub-basins, storage was assumed to be available only by providing special storm water holding facilities at $350 per 1,000 ft^3 of storage which was the most expensive alternative considered.

The fixed costs of providing storm water storage is the sum of the flood plain storage costs and sub-basin 7 storage costs, or $440,000. This figure is less than 3 percent of the total optimal storage cost of approximately $15 million. However, storage within the flood plain alone represents more than 50 percent of the total storm water volume stored.

Table 1. Summary of Model Results - Flood Plain Allocations

Flow and Storage Volumes - 100,000 ft^3

Link i,j	X_{ij}	$\bar{X}_{ij}$	Sub-basin i	R_i	S_i	$\bar{S}_i$
1,J1*	56.4	56.4	1	186.0	130.0	130.0
2,J2	0.0	45.3	2	7.5	7.4	7.4
4,J1	25.1	25.7	3	136.0	48.2	48.2
J1,J2	81.5	82.0	4	25.5	0.0	0.0
J2,3	81.5	127.0	7	96.1	17.0	17.0
3,7*	169.0	169.0	8	39.1	23.3	28.3
14,7	3.5	22.5	9	121.0	0.0	0.0
7,8*	251.0	251.0	10	3.5	3.5	3.5
8,J5	267.0	288.0	11	61.0	1.8	1.8
10,11	0.0	63.6	12	99.0	35.6	35.6
11,J3	59.2	96.1	13	80.3	57.4	57.4
12,J3*	63.4	63.4	14	6.8	3.4	3.4
J3,13	123.0	159.0	15	49.0	69.7	69.7
13,15	145.0	183.0	16	35.9	18.1	18.1
15,J4	125.0	201.0	17	52.4	17.3	17.3
16,J4*	17.8	17.8	18	61.7	25.7	25.7
J4,17	143.0	218.0	19	40.9	0.0	3.1
17,9	178.0	238.0	20	58.5	16.0	16.0
9,18	298.0	314.0				
18,J5*	334.0	334.0				
J5,19	602.0	617.0				
19,J6*	643.0	643.0				
20,J6*	426.0	426.0				
J6,Sink*	685.0	685.0				

*$X_{ij} = \bar{X}_{ij}$

Table 2. Summary of Model Results - Sub-basin Storage and Costs

Sub-basin	Storage Volume Used (100,000 ft^3)	Storage Capacity (100,000 ft^3)	Storage Cost ($)
1	13.8	200.0	484,000
2	86.6	94.0	3,030,000
3	0.0	136.0	0
4	37.4	62.9	1,310,000
7	37.9	37.9	45,000
8	0.0	39.3	0
9	0.0	121.0	0
10	106.0	110.0	3,720,000
11	0.0	61.0	0
12	34.8	134.0	1,220,000
13	11.8	92.1	412,000
14	28.2	35.1	989,000
15	0.0	49.0	0
16	13.2	49.1	462,000
17	0.0	52.4	0
18	0.0	61.7	0
19	0.0	40.9	0
20	87.6	146.0	3,060,000
Flood Plain	483.0	475.0	395,000
Total	940.3	1997.4	15,127,000

These results are given only as an example of how the model can be utilized. In actual practice, the model should be run several times to evaluate the effects of different land use projections and different design storm events. Several runs with varied inputs would provide insight into the sensitivity of the storage allocations and resulting costs. For example, sub-basin 1 at the very top of the drainage system has a greater total potential runoff volume than any other sub-basin (more than twice the average for any sub-basin). What would be the effect of a decision to maintain that area in a more natural state rather than allowing residential development? The resulting cost difference could be significant due to the location of sub-basin 1 and the large increase in potential runoff volume caused by development. Also of interest may be the cost difference of providing the necessary storage for a one year storm rather than the three year event considered in this example.

For this example, the model was run utilizing limited information on the availability and cost of storage. Presently, a great deal more information is available on the cost of storage alternatives. Also, as indicated by the model results, utilization of the flood plain water detention sites and marsh land may provide the most cost-effective solution to controlling storm water runoff. Therefore, more emphasis should be given to considering the availability of natural storage areas within the various sub-basins. Certainly, the model is better utilized when the sub-basin alternative storage costs differ, as they would in evaluating various natural depression sites which might exist throughout the watershed.

The results for this example show that the fixed costs for providing storage within the flood plain and in sub-basin 7 are a small percentage of the total costs. For other situations, this may not be the case. However, if fixed costs are not considered significant, or if they can be reasonably estimated as variable cost, the model can be greatly simplified and more easily solved. The model presented can be easily altered for considering only variable costs by eliminating the integer variables and zero-one inducement constraints.

Conclusions

The mixed integer programming model provides an efficient method for allocating urban storm water runoff among alternative storage sites and can also be used to compare land use and drainage options within an urbanizing watershed where it is important to include fixed charges. The effort required to utilize the decision model as a planning tool is weighted heavily towards data collection; e.g., storage site locations and capacities, hydrologic simulation, land use, and can be used most easily where existing planning has already developed much of the input data requirements. Unless a significant portion of the cost associated with storage alternatives are fixed, the use of a mixed-integer model as presented appears to make the solving of the model more difficult than is necessary. Where all costs can be assumed to be a variable, the model can be greatly simplified by dropping the zero-one variables and constraints. This type of decision model should be used after more simplified approximations have been developed. These simpler approximations should be adequate for most planning studies. More refined procedures such as this mixed integer programming model can be used in specialized cases.

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JOINT USE OF SWMM AND STORM MODELS
FOR PLANNING URBAN SEWER SYSTEMS

Herbert L. Kaufman
Partner
Clinton Bogert Associates
Fort Lee, New Jersey

Fu-Hsiung Lai
Group Supervisor and Project Engineer
Clinton Bogert Associates
Fort Lee, New Jersey

Summary

A joint use of the SWMM and STORM models was demonstrated to provide a tool for sewer system planning which effectively alleviates urban flooding and prevents pollution in the receiving waters. Techniques were developed for projection of runoff characteristics from one drainage district to others for citywide sewer planning.

A concept making use of the characteristics of runoff quantity and quality and interceptor capacity for cost-effective pollution control is described. The pollutants discharged to receiving waters for various interceptor capacities have been comparatively quantified.

Introduction

In the past, concern with storm runoff was mainly over the street and basement flooding and sewers were installed to correct the problem. With the recognition of the pollution problems associated with storm runoff, reduction of pollution reaching natural water bodies has become increasingly desirable.

Elimination of all pollution from wet weather flow could be prohibitively expensive nor is it necessary to prevent damage to the environment. The marginal benefit received by society usually diminishes with each additional increment of pollution abatement facility provided. Hence, there exists an optimal level of expenditure for pollution control that society should plan to provide. The determination of this optimal level depends upon many factors, including (1) the degree of flood protection justified, (2) the characteristics of real storm runoff, (3) the combined sewage quantity and quality and the character of the receiving waters.

Because of the complex nature of the urban rainfall-runoff and pollutant accumulation-washout-transport processes, and the many management alternatives, reliance on computer models to assist in the system simulation becomes advantageous. There are at least 16 mathematical models developed which permit the planning of sewer systems to alleviate urban flooding, and prevent pollution in the receiving waters.[1,2,3] Of these models, the EPA Storm Water Management Model,[4] frequently abbreviated "SWMM" and the Corps of Engineers' Storage, Treatment, and Overflow Model[5], abbreviated as "STORM", are probably the most useful and comprehensive for urban sewer system design and planning. These two models consider both runoff quantity and quality.

The SWMM Model can simulate rainfall-runoff processes in fine scale, both spatially and temporally, and route storm runoff quantity and quality from individual catchments and subcatchments through a sewer pipe network. It can be used to analyze or design a sewer system for an actual or synthetic storm event. It can also be adapted for planning studies. The STORM Model can economically analyze hourly runoff quantity and quality for long-term precipitation records, based on such parameters as percent imperviousness and land use. It has been used to evaluate the effectiveness of storage and treatment facilities for overflow pollution control[6]. Unlike the SWMM Model, which considers overland and sewer flow routing, no such routing is made in the STORM Model.

The existing SWMM Model requires the use of short time intervals (minutes) for routing runoff quantity and quality. It cannot be used for simulation or analysis based on long-term precipitation data. The STORM Model, while it can provide a time history of overflows for a given storage and treatment capacity for continuous rainfall data recorded hourly, does not model the collection and conveyance system which is an essential part in a cost-effective study.

The advantage of joint use of the SWMM and STORM Models has been demonstrated in the current study to establish the optimum design for possible alternative sewer systems for the City of Elizabeth, New Jersey. This paper will attempt to demonstrate the advantage of using these two models, somewhat modified, jointly for flood control and pollution abatement.

The design of sewer system components was based on (1) protecting the urban area from flooding by a storm with a 5-year return frequency, and (2) providing interceptor, storage and treatment facilities to optimally minimize the frequency of, and the pollutants in, the untreated overflows. The amount and frequency of overflow that can be tolerated would depend upon the characteristics of the overflow and the assimilating capacity of receiving waters. As far as the environmental effects are concerned, the more frequently occurring rainfalls appear to cause greater impact on the receiving waters than the more intensive storms with return frequencies greater than one-year. Hence, design of storage and treatment facilities and interceptor sewers would be based on real rainstorms which could be no more intense than a one-year return frequency storm.

Description of Study Area

The study area consists of the City of Elizabeth, New Jersey. Data developed through modeling of Drainage District A was through correlation of STORM and SWMM applied to planning for the entire City. Figure 1 shows the location of the study area.

The 4400 acres of urban development are served by 25 drainage districts. The population of the City is close to saturation and is expected to have only a moderate future growth. The land uses in District A are predominantly residential (about 90 percent), with some neighborhood commercial (about 5 percent) and small industrial areas (about 3 percent). The relevant land use data are shown in Table 1. The district has an estimated population of 16,500, or about 25 persons per acre. Its impervious area equals 47 percent of the total.

The existing sewer system in the City is of the combined type. The sewers are old and undersized, as

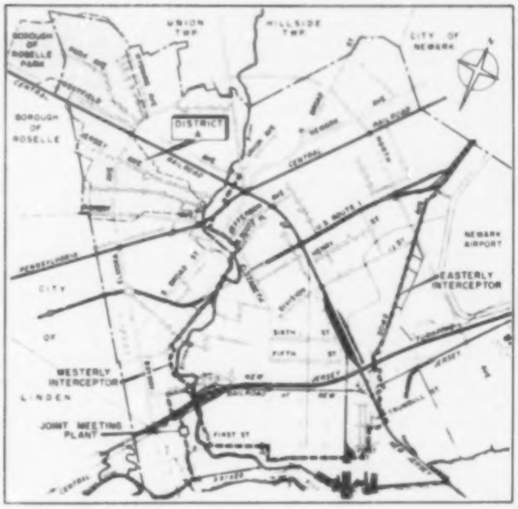

FIGURE 1. Study Area

TABLE 1

DRAINAGE DISTRICT A LAND USE DATA

Land Use	% of Area	% Impervious	Curb Length (Ft/Acre)
Single Family	71.7	43	413.
Multiple Family	18.2	50	298.
Commercial	5.3	80	283.
Industrial	2.8	80	216.
Open Space	2.0	19	296.

is the Westerly Interceptor which parallels the Elizabeth River. There are numerous complaints of street and basement flooding. Overflows to the Elizabeth River are frequent.

Secondary treatment facilities are now under construction at the Joint Meeting Plant. The City has allocated to it a peak wet weather flow capacity of 40 million gallons per day (mgd). The Corps of Engineers has also planned a diked storage area, with a total capacity of about 21 million gallons, along the Elizabeth River near the Joint Meeting Plant.

The Elizabeth River is tidal from its mouth to the Penn Central Railroad. The river, which drains about 23 square miles, does not provide adequate dilution for the untreated initial overflows of combined sewage.

Modification of SWMM and STORM Programs

In addition to continuous updating of the models as revisions become available, both models were modified. The SWMM program was modified to allow design capability with gutter pipes surcharged. This eliminated revising the input sewer dimension for the elimination of such surcharge.

The STORM program was modified to include a dry weather flow routine for simulation of combined sewage overflows. Input data allow diurnal hourly variation of dry weather flow quantity and quality for various land uses. A copy of the program changes has been forwarded to the Hydrologic Engineering Center (HEC) of the Army Corps of Engineers for incorporation in the new version of STORM to be released.

Quantity and Quality Considerations

Differences between SWMM and STORM in the consideration of storm runoff quantity and quality are worth noting.

Quantity

In STORM, runoff volume from the watershed is calculated on an hourly basis as a function of rainfall plus snowmelt. Losses of rainfall and/or snowmelt volume due to infiltration in the watershed are accounted for by the use of a runoff coefficient C. C is derived from two basic coefficients, C_1 and C_2. C_1 represents the runoff coefficient for pervious areas and C_2 for impervious areas. For a given watershed, knowing the land uses, the amount of depression storage averaged over the watershed and the amount of rainfall and snowmelt, C can be calculated from C_1 and C_2 to determine the amount of runoff. There is no runoff from the watershed until the detention storage, which is uniformly applied to the entire watershed, is filled.

In SWMM, runoff volume over a fine time interval is made by using a number of overland flow elements to simulate the initial collection processes. The amount of runoff from pervious and impervious areas is separately considered. Infiltration loss from pervious areas is computed using Horton's equation. In addition, rainfall on a certain percent of impervious areas results in immediate runoff and enters the sewer system without time delay and loss of volume. This is true regardless of the amount of rainfall since dwellings, such as those in Elizabeth with pitched roofs, have roof drains directly connected to a street gutter.

SWMM uses a more valid concept of the hydraulics of rainfall-runoff processes than STORM. Parameters required for SWMM Model can be reasonably estimated. The model has been applied to a number of watershed in the United States[7,8] and the accuracy of the runoff quantity computations has been relatively good. If a watershed is segmented properly, SWMM can be used for runoff prediction in urban areas.

The significant advantage of STORM is its ability to analyze input from long-term rainfall records to evaluate overall rainfall pattern effects.

Quality

Neglecting land surface erosion and dry weather flow, both SWMM and STORM compute street pollutant washout by storm runoff according to the amount of dust and dirt accumulated along the street curbs prior to the occurrence of a storm. From the total pounds of dust and dirt washout, the pollutant components such as suspended solids (SS) and BOD are computed either for the available local data or from specified default values. In study areas where quantity and quality data are not available for evaluating pollutant parameters, default values specified to either program could be used.

Both SWMM and STORM use the same default values for most of the pollutant calculations except for SS and BOD. The value used by SWMM for suspended solids is about ten times and for BOD, about 5 times that used by STORM. More discussions and comparisons of runoff quality computation can be found in the reference[9].

As SWMM is an event simulator and STORM an analytical tool for long-term rainfall records, the computations of street dust and dirt accumulation with dry days and street sweeping are different. Figure 2 shows that pollutant accumulation as computed by SWMM increases monotonically with the number of antecedent dry days for an assumed seven-day street sweeping interval. The pollutant accumulation calculated by STORM indicated periodical fluctuation of SS accumulation at the street curb reflecting the effect of street cleaning frequency and the number of dry days since the last street cleaning. In SWMM, additional accumulation of dust and dirt on the street curb is assumed to be equal to the maximum accumulation for the period between successive street sweeping. It does not credit the cleaning effects of street sweeping. Recognition of this difference is significant when making comparison of runoff quality from a single storm event with two models.

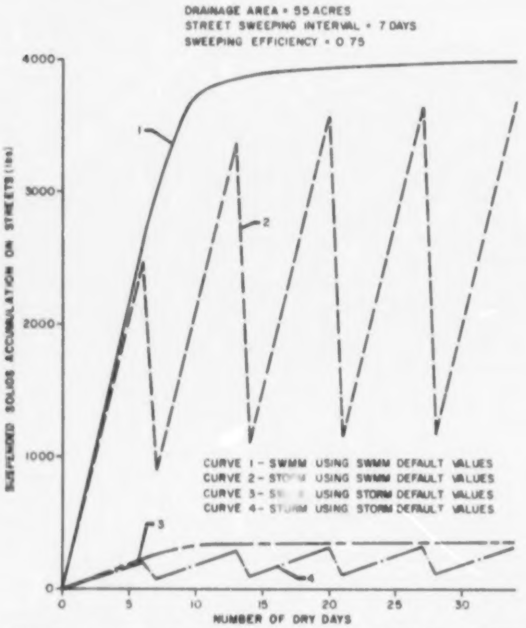

FIGURE 2. Street SS Accumulation, SWMM Vs. STORM

As the use of SWMM generally requires fine time interval for rainfall input and flow routing, rainfall intensity during the course of a rainstorm may be greater than hourly rainfall intensity required for STORM. Higher intensity of rainfall would mean greater pollutant washout from streets.

Calibration of STORM Runoff Coefficient

Runoff coefficients, C_1 and C_2 respectively, for pervious and impervious areas, used in STORM, were calibrated using data generated by SWMM in District A. These coefficients were applied to other drainage districts in the City to obtain runoff volume from synthetic or real rainstorms.

For use of SWMM, District A was subdivided into 279 subcatchments with an average area of 2.3 acres. The surface runoff from these subcatchments drains into 139 gutter pipes and subsequently to 32 trunk sewers. The downstream end of the sewer system connects to the Westerly Interceptor.

The following assumptions were made in the calibration of C_1 and C_2:

1. Surface runoff data was generated by a program adapted from the SWMM RUNOFF Block without gutter routing. This is consistent with the STORM program, in which the effect of gutter flow is not considered.

2. The depression storage capacities for pervious and impervious areas used in SWMM were 0.25 and 0.062 inches, respectively. 25 percent of the impervious area was assumed to have no detention storage. The equivalent depression storage for District A was computed as 0.155 inches, based upon 47 percent of the area being impervious.

3. The infiltration capacity curve shown in Figure 3 was used in SWMM to account for the infiltration loss. A maximum rate of infiltration of 3.0 in/hr, a minimum of 0.28 in/hr, and a decay rate of 0.00138/sec was used. The antecedent conditions for rainfall events were such that the infiltration curve specified applied. Assumption for STORM is that the depression storage capacity of 0.155 inches is available prior to the beginning of the rainfall event.

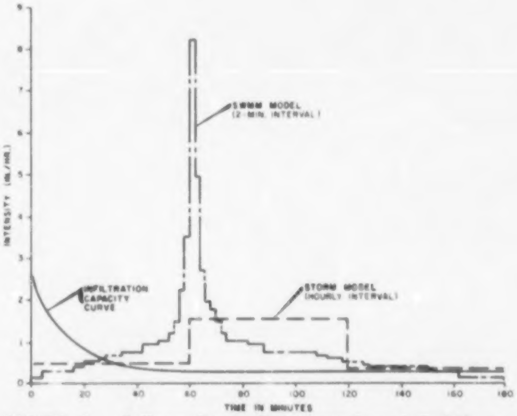

FIGURE 3. 5-Year Storm Hyetograph and Infiltration Curve

4. A typical rainfall event is assumed to have three-hour duration and an intermediate pattern similar to the 5-year design storm with hourly interval as shown in Figure 3. In fact, use of 2-minute hyetograph or of 1-hour hyetograph results in little difference in total surface runoff volume from 3-hour rainfall event. The 5-year storm has the average 1-hour, 2-hour, and 3-hour rainfall intensities of 1.6, 1.05 and 0.81 inches per hour respectively.

5. The runoff coefficient, C_2, for the impervious area, was set equal to 1.0, since there is no infiltration loss for an impervious area and the depression storage is accounted for separately.

The runoff coefficient for pervious area C_1 is calibrated so that the 3-hour storm runoff volume computed with the adapted SWMM program is the same as that computed with the STORM program. The calibrated C_1 values are shown in Figure 4 as a function of 3-hour rainfalls. As anticipated, C_1 increases with an increase in the amount of rainfall (or average rainfall intensity) over the specified duration. For the

5-year design storm used in the study, with a total rainfall of 2.43 inches or an average intensity of 0.81 inches per hour, a C_1 value of 0.55 would be appropriate. For other rainfall amounts, such as 0.6, 1.38, and 4.86 inches (or intensities 0.2, 0.46 and 1.62 inches per hour respectively), the appropriate C_1 values are 0.25, 0.3 and 0.78. 0.6 and 1.38 inches of rainfall respectively correspond to a storm return interval of 1.3 month and 1 year, based on the analysis of hourly rainfall data recorded at the Newark International Airport from 1963 to 1974. 85 percent of rainfall during that period has an amount less than 0.6 inches.

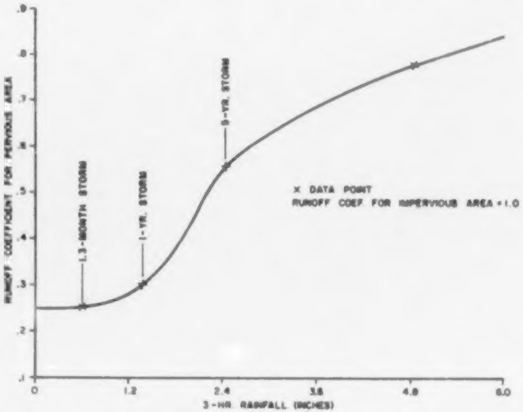

FIGURE 4. STORM Runoff Coefficient Vs. Rainfall

Considering that the runoff coefficient, C_1, increases with the amount of rainfall and STORM assumes a constant runoff coefficient for the entire time span of records to be simulated regardless of the rainfall volume or intensity, a C_1 value of 0.25 was proposed for the simulation of long-term rainfall records for overflow pollutional evaluation. Reducing C_1 value to 0.15 results in a nine percent reduction in the mass volume of overland flow from District A using 12-year data. The amount of pollutant washout from streets is independent of C_1. It therefore is apparent that the selected C_1 value of 0.25 should provide sufficiently consistent results from the STORM program to permit valid engineering evaluation.

Generation of 5-Year Design Storm Runoff Hydrograph

As mentioned earlier, the City has 25 drainage districts with District A the largest in area. Citywide planning requires development of a runoff hydrograph and pollutograph from each drainage basin for storms of interest. These runoff hydrographs and pollutographs are required for cost effective sizing of intercepting sewers, storage and treatment facilities. Upstream collection sewers in each drainage district are adequately sized so that street and/or basement flooding would be prevented for a design storm with a 5-year return interval.

A 5-year storm runoff hydrograph for all drainage districts could be obtained by making a detailed sewer layout and by segmenting the catchment and preparing land use data in each district. The amount of work involved is usually more than required or justified for master planning. An alternative is to make a detailed study in one district for projection to other drainage districts.

Storm runoff and sewer routing in District A were analyzed using SWMM. Overland and gutter flows were analyzed with the SWMM RUNOFF Block and trunk sewer flow with or without sanitary wastes with the SWMM TRANSPORT Block. Catchment and land use data were prepared to the necessary detail for accuracy. Although there are existing combined sewers in District A, they are totally inadequate in size. The new sewer system was designed to convey the total 5-year storm runoff. Existing sewer data, however, were used in preparing sewer layout, slope, and other pertinent sewer information.

The two primary factors governing the shape and rate of the routed hydrograph for a given drainage basin are area and percent of imperviousness. The area affects mainly the extent of flow attenuation and the peaking time of a hydrograph. The land use, and consequently percent of imperviousness, affects mainly the runoff volume. Normalized hydrographs, based on information developed for District A, were used to determine hydrographs for other drainage districts.

Comparison of the normalized hydrographs within the range of drainage areas to be analyzed showed the effect on the hydrograph shape of percent of imperviousness or equivalently, the land uses to be insignificant. To represent the variation of hydrograph shape with drainage area, five normalized hydrographs were used. Two of the normalized hydrographs are shown in Figure 5, one for a drainage area greater than 500 acres and one for a drainage area less than 150 acres. Figure 5 also shows the larger drainage area to have a hydrograph with greater spread and delayed peaking time.

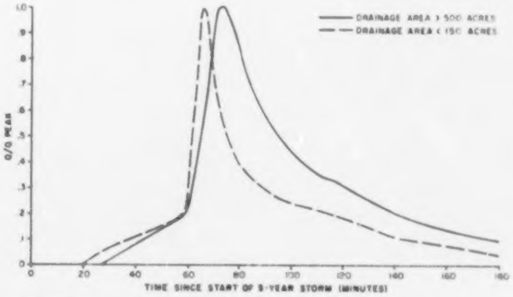

FIGURE 5. Normalized Hydrographs

The 5-year storm runoff volume in drainage districts other than District A was obtained with the STORM program, using the calibrated runoff coefficient 0.55 for pervious area and 1.0 for impervious area and the available land use data. Dividing the runoff volume by the integrated area enclosed by the appropriate normalized hydrograph permitted estimation of the outflow hydrograph.

Figure 6 shows three computed outflow hydrographs expressed in cubic foot per second per acre. It illustrates the effect of drainage area combined with the percent of imperviousness on the shape and peak runoff rate per acre.

Planning Interceptors For Pollution Control

Conveyance of 5-year storm runoff by interceptors to storage for later treatment would not only be prohibitively costly but also is not required to prevent pollution. Pollutional effects from a storm occurring, on the average, once in five years, would not cause as much damage as a storm occurring monthly.

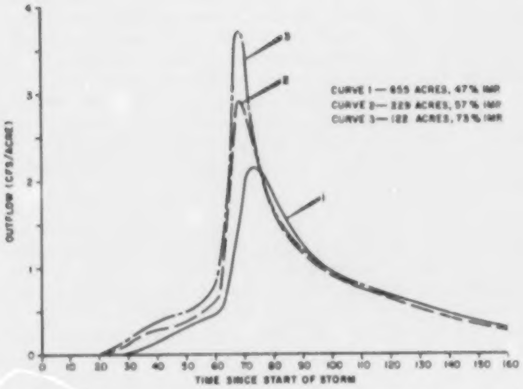

FIGURE 6. Computed Outflow Hydrographs

To determine the quantity of runoff to be stored and treated, the characteristics of storm runoff and combined sewage quantity and quality were investigated.

SWMM was used to obtain the storm runoff and combined sewage quantity and quality from District A. Average conditions of four antecedent dry days, a seven-day street sweeping interval and 75 percent sweeping efficiency were assumed. Quantity and quality of dry weather flow used are in conformance with the EPA Study[10]. In computing suspended solids from street dust and dirt washout, STORM default values were used.

In addition to the 5-year storm, runoff from a 1-year and a 1.3-month storm was analyzed. The rainfall characteristics of these two storms were obtained using a partial duration series analysis of hourly data for a 12 year period. They were also assumed to have the same pattern as the 5-year storm. Figure 7 shows the 5-year storm hydrograph and pollutographs from District A. Runoff from 1-year and 1.3-month storms has characteristics similar to the 5-year storm, with the difference basically in the magnitude of flow and pollutant loading.

Curve A of Figure 7 is the outflow hydrograph which maintains a relative low value until one hour after the rainfall starts. Curves B and C respectively show the suspended solids (SS) concentration (mg/l) and rate (pounds per minute) of combined sewage outflow. The SS concentration of storm runoff without sanitary wastes is shown in Curve D.

Curve C illustrates the existence of two flushes in a combined sewer. The first flush ends about 50 minutes from the start of the storm when the flow rate is computed at 207 cfs and the concentration of suspended solids is 25 mg/l. This flush is mainly attributed to the deposit of solids in combined sewers from sanitary wastes during dry days. The second flush ends about 40 minutes later when the flow rate is estimated at 850 cfs. This flush represents mainly the street pollutant washout. To contain the first flush, a storage volume equivalent to 0.063 inches of rainfall over the entire area of District A is required. For containment of the second flush, however, 0.906 inches of storage would be necessary.

Curve B, which sets forth the concentration of the pollutant discharge, permits drawing significant conclusions. There is only one peak polluting discharge which ends about 56 minutes from the beginning of rainfall. The peak polluting discharge is defined as one containing a SS concentration of more than 20 mg/l. The flow rate is computed as 249 cfs at that time. The storage volume required to contain this first flush is 0.098 inches over the entire drainage

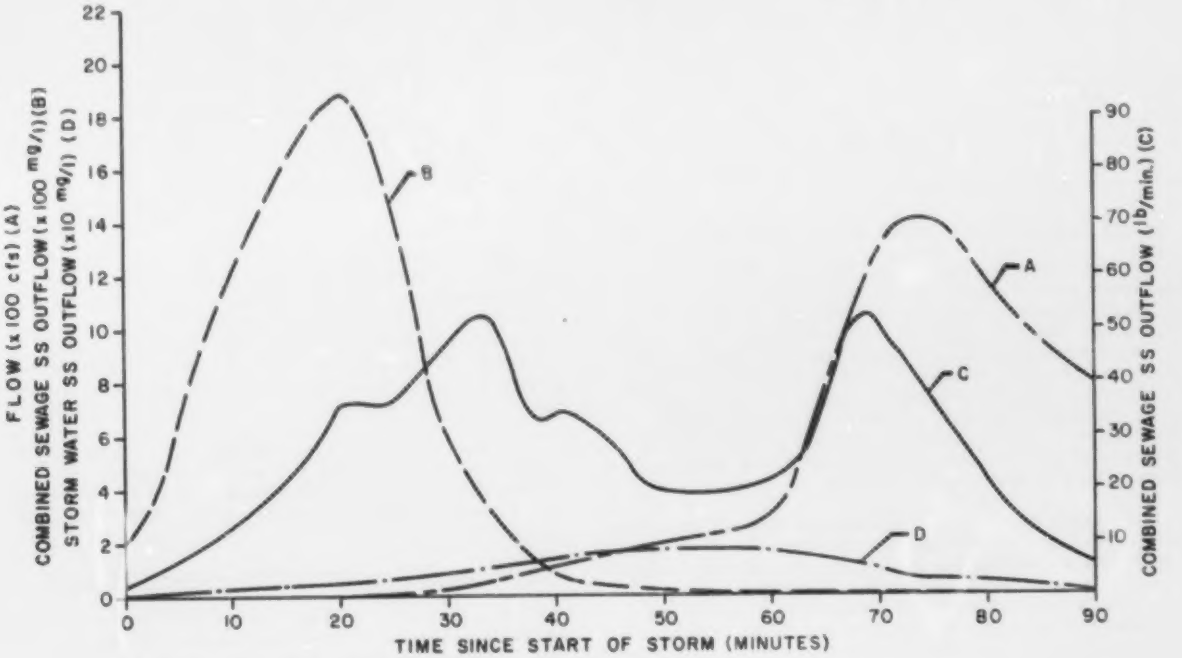

FIGURE 7. 5-Year Storm Hydrograph and Pollutographs

basin. Hence, because of the low concentration of pollutants found in the second flush shown in Curve C, its containment does not appear justified.

For containment of the first flush (as previously defined), from the 1-year storm, the magnitude of intercepted flows from District A was computed as 549 cfs and the required storage equal to 0.144 inches. If the criteria for the first flush limit is increased to 22 mg/l of SS, the design requirement reduces to 153 cfs and 0.055 inches. For the 1.3-month storm, the computed flows are 213 cfs and a storage of .103 inches for the defined first flush limitation.

Dividing regulated flows of 35, 153, 207, 249, and 549 cfs by the unregulated 5-year storm peak outflow of 1406 cfs, the ratios of regulated peak outflow to unregulated 5-year storm peak outflow are 0.0249, 0.1088, 0.1472, 0.1771, and 0.3905 respectively. Applying these ratios to the 5-year storm runoff hydrographs for other drainage districts, the inflow hydrographs to interceptors were obtained for various degrees of runoff control.

Runoff from the City's twenty-five drainage districts was assumed to drain into interceptors at 14 inlet locations. The SWMM Transport Block was used for sizing of interceptors for conveyance of regulated flow to a storage basin near the treatment plant.

STORM was also used for Drainage District A to analyze the 12-year (1963-1974) hourly precipitation data to obtain annual statistics of overflow events and pollutional loadings for various amounts of flow intercepted for treatment.

Figure 8 shows at various ratios of interceptor capacity the (1) combined sewage SS concentration discharged to receiving waters, (2) annual number of overflow events from District A, and (3) cost of pumping facilities for storage and interceptor facilities. Data for storms with a return frequency of 5 years, 1 year and 1.3 months is shown. Other costs do not vary with the ratio of interceptor capacity to peak design storm flow.

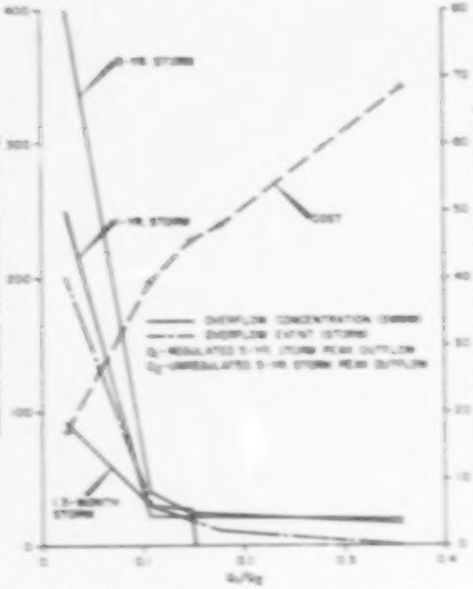

FIGURE 8. Cost-Effective Pollution Control Considerations

For interceptor capacity to peak flow ratio of 0.0249, inadequate control of pollution would be experienced.

At a ratio of 0.1088, the cost is estimated at $39.4 million, with discharge SS concentration of 40, 22, and 30 mg/l respectively for the 5-year, 1-year and 1.3-month storms. The number of annual overflow events extending one hour or more is 6.6. These events would discharge a total of 2702 lbs. of SS and 620 lbs. of BOD. An increase of the ratio to 0.1472 increases costs by 15 percent to $45.5 million, but reduces the overflow SS concentrations to 25, 21.4 and 26.7 mg/l for the three storms respectively and the number of annual overflow events of one hour or more duration to 3.8. These would contain a total of 1150 lbs. of SS and 260 lbs. of BOD. However, short duration overflows would still occur with the 1.3-month storm. Further increase of the ratio to 0.1991 would increase cost by less than 5 percent to $47.6 million but would eliminate overflow from 1.3-month storm. The number of annual overflow events of one hour or more would be 2.3. Further increase in the ratio and its capital cost increment would result in insignificant return in pollution control. Conveyance of uncontrolled 5-year storm runoff would cost as much as $121 million.

Based on the above discussions, the range of cost-effective interceptor flows for pollution control would be from 10 to 18 percent of the peak 5-year storm runoff with the planned storage and treatment capacity available in Elizabeth.

Conclusions

A joint use of the SWMM and STORM models was demonstrated to provide a useful tool for planning sewer systems for cost-effective flood control and pollution abatement.

The study shows that intercepting flows from 10 to 18 percent of the peak 5-year design storm runoff would be within the range of being cost-effective and would adequately intercept the most significant part of runoff pollutants.

Acknowledgements

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SIMULATION OF AGRICULTURAL RUNOFF

Anthony S. Donigian, Jr.
Hydrocomp, Inc. Palo Alto, CA

Norman H. Crawford
Hydrocomp, Inc. Palo Alto, CA

Abstract

The Agricultural Runoff Management (ARM) Model described in this paper simulated runoff, snow accumulation and melt, sediment loss, pesticide-soil interactions, and soil nutrient transformations on small agricultural watersheds. The results of Model testing for simulation of runoff, sediment, and pesticide loss are presented to demonstrate possible uses of the ARM Model as a tool for evaluating the water quality impact of agricultural practicies.

Introduction

The development of models to simulate the water quality impact of nonpoint source pollutants is receiving considerable attention by the engineering and scientific community. One of the major reasons for this interest is the passage of the Federal Water Pollution Control Act Amendments of 1972, specifically requiring the evaluation of the contribution of nonpoint source pollution to overall water quality. This paper describes a modeling effort whose goal is the simulation of water quality resulting from agricultural lands. The beginnings of this research modeling effort date from 1971 when the U.S. Environmental Protection Agency, through the direction of the Environmental Research Laboratory in Athens, Georgia (ERL-Athens), sponsored the development and initial testing of the Pesticide Transport and Runoff (PTR) Model (1). The Agricultural Runoff Management (ARM) Model discussed in this paper is the combined result of further model testing and refinement, algorithm modifications, and inclusion of additional capabilities not present in the PTR Model. The ultimate goal of the continuing ARM Model development effort is the establishment of a methodology and a tool for the evaluation of the efficacy of management practices to control the loss of sediment, pesticides, nutrients, and other nonpoint pollutants from agricultural lands.

Modeling Philosophy

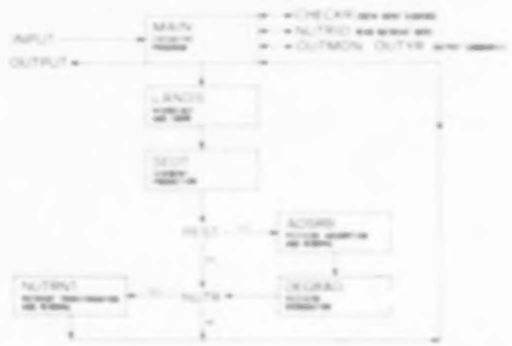
The guiding philosophy of the modeling effort is to represent, in mathematical form, the physical processes occurring in the transport of nonpoint pollutants. The hydrologic and water quality related processes occurring on the land surface (and in the soil profile) are continuous in nature; hence, continuous simulation is critical to the accurate representation of these physical processes. Although nonpoint source pollution from the land surface takes place only during runoff-producing events, the status of the soil moisture and the pollutant prior to the event is a major determinant of the amount of runoff and pollutants that can reach the stream during the event. In turn, the soil moisture and pollutant status prior to the event is the result of processes that occur between events. Cultivation and tillage practices, pesticide and fertilizer applications, pesticide degradation and nutrient transformations, all critically affect the mass of pollutant that can enter the aquatic environment during a runoff-producing event. Models that simulate only single events cannot accurately evaluate agricultural land management practices since between-event processes are ignored. Although all between-event processes cannot be precisely described at the present state of technology, continuous simulation provides a sound framework for their approximation and for further research into their quantification.

When modeling nonpoint source pollution, the above stated philosophy is joined by the fact that the transport mechanisms of such pollutants are universal. Whether the pollutants originate from pervious or impervious lands, from agricultural or urban areas, or from natural or developed lands, the major transport modes of runoff and sediment loss are operative. (Wind transport may be significant in some areas, but its importance relative to runoff and sediment loss is usually small.) In this way, the simulation of nonpoint source pollution is analogous to a three-layered pyramid. The basic foundation of the pyramid is the hydrology of the watershed. Without accurate simulation of runoff, modeling nonpoint pollutants is practically impossible. Sediment loss simulation, the second layer of the pyramid, follows in sequence the hydrologic modeling. Although highly complex and variable in nature, sediment modeling provides the other critical transport mechanism. The pinnacle or final layer of the pyramid is the interaction of various pollutants with sediment loss and runoff, resulting in the overall transport simulation of nonpoint source pollutants.

The Agricultural Runoff Management (ARM) Model

The ARM Model simulates runoff (including snow accumulation and melt), sediment, pesticides, and nutrient contributions to stream channels from both surface and subsurface sources. No channel routing procedures are included. Thus, the Model is applicable to watersheds that are small enough that channel processes and transformations can be assumed negligible. Although the limiting area will vary with climatic and topographic characteristics, watersheds greater than one to two square miles are approaching the upper limit of applicability of the ARM Model. Channel processes will significantly affect the water quality in larger watersheds.

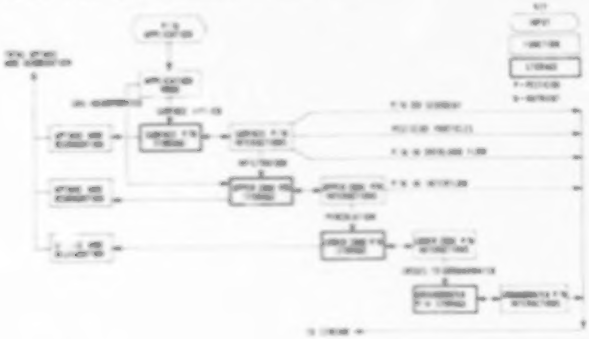
Figure 1 demonstrates the general structure and operation of the ARM Model. The major components of the Model individually simulate the hydrologic response (LANDS) of the watershed, sediment production (SEDT), pesticide adsorption/desorption (ADSRB), pesticide degradation (DEGRAD), and nutrient transformations (NUTRNT). The executive routine, MAIN, controls the overall execution of the program; calling subroutines at proper intervals, transferring information between routines, and performing the necessary input and output functions.



In order to simulate vertical movement and transformations of pesticides and nutrients in the soil profile, specific soil zones (and depths) are established so that the total soil mass in each zone can be specified. Total soil mass is a necessary ingredient in the pesticide adsorption/desorption reactions and nutrient transformations. The vertical soil zones simulated in the ARM Model include the surface, upper, lower, and groundwater zones. The depths of the surface and upper soil zones are specified by the Model input parameters, and are generally 3-6 mm and 75-150 mm, respectively. The upper zone depth corresponds to the depth of incorporation of soil-incorporated chemicals. It also indicates the depth used to calculate the mass of soil in the upper zone whether agricultural chemicals are soil-incorporated or surface-applied. The depths of the surface and lower zones are important because the active surface zone is crucial to the washoff and degradation of agricultural chemicals, while the extent of the lower zone determines to what degree soluble pollutants will contaminate the groundwater. The lower zone depth is presently specified as 1.8 meters (6 feet). However, the zonal depths will vary with the geology and topography of the watershed. Further evaluation of these zones is presently in progress.

The transport and vertical movement of pesticides and nutrients, as conceived in the ARM Model, is indicated in Figure 2. Pollutant contributions to the stream can occur from the surface zone, the upper zone, and the groundwater zone. Surface runoff is the major transport mechanism carrying dissolved chemicals, pesticide particles, or sediment and adsorbed chemicals. The interflow component of runoff can transport dissolved pesticides or nutrients occurring in the upper zone. Vertical chemical movement between the soil zones is the result of infiltrating and percolating water. From the surface, upper, and lower zones, uptake and transformation of nutrients and degradation of pesticides is allowed. On the watersheds tested, the groundwater zone has been considered a sink for deep percolating chemicals since the groundwater flow contribution has been negligible. However, on larger watersheds this contribution could be significant.

Figure 2. Pesticide and nutrient movement in the ARM model



Model Algorithms

The algorithms, or equations, used to describe the processes simulated by the ARM Model are fully discussed in the final project report (2). A brief presentation of the general methodology is included here.

Hydrology

Hydrologic simulation by the LANDS subprogram is derived from modifications of the Stanford Watershed Model (3) and the Hydrocomp Simulation Program (4). Through a set of mathematical functions, LANDS simulates continuously the major components of the hydrologic cycle, including interception, surface runoff, interflow, infiltration, and percolation to groundwater. In addition, energy balance calculations are performed to simulate the processes of snow accumulation and melt. Various publications have previously described the hydrologic (1, 3, 4, 5) and snowmelt algorithms (2, 4, 5).

Sediment

The algorithms for simulating soil loss, or erosion, were initially derived from research by Negev at Stanford University (6) and have been subsequently influenced by the work of Meyer and Wischmeier (7), Onstad and Foster (8), and Fleming and Fahmy (9).

Although Negev simulated the entire spectrum of the erosion process, only sheet and rill erosion were included in the ARM Model. The two component processes of sheet and rill erosion pertain to (1) detachment of soil fines (generally the silt and clay fraction) by raindrop and impact, and (2) pick-up and transport of soil fines by overland flow. These processes are represented as follows:

Soil fines detachment:

$$RER(t) = (1 - COVER(T))*KRER*PR(t)^{JRER} \qquad (1)$$

Soil fines transport:

$$SER(t) = KSER*OVQ(t)^{JSER}, \text{ for } SER(t) \leq SRER(t) \qquad (2)$$

$$SER(t) = SRER(t), \text{ for } SER(t) > SRER(t) \qquad (3)$$

$$ERSN(t) = SER(t)*F \qquad (4)$$

where

RER(t) = soil fines detached during time interval t, tonnes/ha
COVER(T) = fraction of vegetal cover as a function of time, T, within the growing season
KRER = detachment coefficient for soil properties
PR(t) = precipitation during the time interval, mm
JRER = exponent for soil detachment
SER(t) = fines transport by overland flow, tonnes/ha
JSER = exponent for fines transport by overland flow
KSER = coefficient of transport
SRER = reservoir of soil fines at the beginning of time interval, t, tonnes/ha
OVQ(t) = overland flow occurring during the time interval, t, mm
F = fraction of overland flow reaching the stream during the time interval, t
ERSN(t) = sediment loss to the stream during the time interval, t, tonnes/ha

In the operation of the algorithms, the soil fines detachment (RER) during each time (5 or 15 minutes) interval is calculated by Equation 1 and added to the total fines storage or reservoir (SRER). Next, the total transport capacity of the overland flow (SER) is determined by Equation 2. Sediment is assumed to be transported at capacity if sufficient fines are available, otherwise the amount of fines in transport is limited by the fines storage, SRER (Equation 3). The sediment loss to the waterway in the time interval is calculated in Equation 4 by the fraction of total overland flow that reaches the stream. A land surface flow routing technique (1, 4, 5) determines the overland flow contribution to the stream in each time interval. After the fines storage (SRER) is reduced by the actual sediment loss to the stream (ERSN), the algorithms are ready for simulation of the next time interval. Thus, the sediment that doesn't reach the stream is returned to the fines storage and is available for transport in the next time interval. The methodology attempts to represent the major processes of importance in soil erosion so that the impact of land management practices (e.g. tillage, terracing, mulching, etc.) can be specified by their effects on the sediment parameters.

Pesticides

The process of pesticide adsorption/desorption onto sediment particles is a major determinant of the amount of pesticide loss that will occur. This process establishes the division of available pesticide between the water and sediment phases, and thus specifies the amounts of pesticide transported in solution and on sediment. The algorithm employed to simulate this process in the ARM Model is described as follows:

$$X/M = KC^{1/N} + F/M \qquad (5)$$

where X/M = pesticide adsorbed per unit soil, µg/gm
F/M = pesticide adsorbed in permanent fixed state per unit soil. F/M is less than or equal to FP/M, where FP/M is the permanent fixed capacity of soil in µg/gm for pesticide. This can be approximated by the cation or anion exchange capacity for that particular soil type.
C = equilibruim pesticide concentration in solution, mg/l
N = exponent
K = coefficient

Basically this algorithm is comprised of an empirical term, F/M, plus the standard Freundlich single-valued (SV) adsorption/desorption isotherm (solid line in Figure 3). The empirical term, F/M, accounts for pesticides that are permanently adsorbed to soil particles and will not desorb under repeated washing. As indicated in Figure 3, the available pesticide must exceed the capacity of the soil to permanently adsorb pesticides before the adsorption/desorption equilibrium is operative. Thus the pesticide concentration on soil particles must exceed FP/M before the equilibrium soil and solution pesticide concentrations are evaluated by the Freundlich curve. An in-depth description and discussion of the underlying assumptions is presented in the PTR Model report (1).

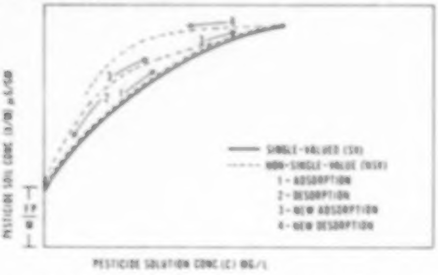


Figure 3. Adsorption/desorption algorithms in the ARM model

The ARM Model includes an option to use a non-single-valued (NSV) adsorption/ desorption function because research has indicated that the assumption of single-valued adsorption/desorption (Figure 3) is not valid for many pesticides (10, 11, 12). In these cases, the adsorption and desorption processes would follow different curves, as indicated by the dashed lines in Figure 3. The NSV algorithm utilizes the above SV algorithm (solid line) as a base from which different desorption curves are calculated. The form of the desorption curve is identical to Equation 5 except that K and N values are replaced by K' and N' respectively. The prime denotes the desorption process. The user specifies the N' value as an input parameter (NP), and the ARM Model calculates K' as a function of the adsorption/desorption parameters (K, N, N') and the pesticide solution concentration (12). The calculation is performed whenever the desorption process is initiated. The end result is desorption curves emanating from the base SV adsorption curve as shown in Figure 3. Thus the NSV function simulates higher pesticide concentrations on sediment than the SV function in order to represent the irreversibility of the adsorption process.

Attenuation of the applied pesticide, through volatilization and degradation processes, is also critical to the accurate simulation of pesticide transport from the land surface. These processes are not well understood and are topics of continuing research. The ARM Model includes a simple daily first-order degradation factor (user input) to approximate the reduction in the amount of pesticide that can be transported anytime during the growing season. More sophisticated degradation models are presently being investigated for addition to the ARM Model.

Nutrients

Nutrient simulation in the ARM Model attempts to represent the reactions of nitrogen and phosphorus compounds in the soil profile as a basis for predicting the nutrient content of agricultural runoff. The nutrient model assumes first-order reaction rates and is derived from work by Mehran and Tanji (13), and Hagin and Amberger (14). The processes simulated include immobilization, mineralization, nitrification/denitrification, plant uptake, and adsorption/desorption. The model is presently being refined and tested on field data. The final project report (2) includes a complete description of the nutrient model and discussions of the component processes.

ARM Model Testing and Simulation Results

The ARM Model development effort is supported by an extensive data collection and analysis program sponsored by the Environmental Protection Agency's Environmental Research Laboratory in Athens, Georgia (ERL-Athens). Test watersheds located in Georgia and Michigan, ranging from 0.6 to 2.7 hectares, have been instrumented for the continuous monitoring and sampling of runoff and sediment. Collected samples are refrigerated on site and later analyzed for pesticide and nutrient content. In addition, meteorologic conditions are continuously monitored and soil core samples are taken and analyzed immediately following application and periodically throughout the growing season.

Model testing for runoff, sediment loss, and pesticide loss was completed on one year of data (January 1973-December 1973) from the P1 and P3 watersheds in Watkinsville, Georgia. P1 (2.70 ha) is a natural watershed while P3 (1.26 ha) is a terraced watershed with a grass waterway. Both watersheds received identical management practices during 1973: minimum tillage was employed, soybeans were planted, and the herbicides paraquat (1,1'-dimethyl-4,4-bipyridinium ion), diphenamid (N, N-dimethyl-2, 2-diphenylacetamide), and trifluralin (α, α, α -trifluoro-2, 6-dinitro-N, N-dipropyl-p-toluidine) were applied at 1.1, 3.4 and 1.1 kg/ha, respectively. Pesticide simulations were performed for paraquat and diphenamid.

The monthly simulation results on the P1 watershed (Figures 4 and 5) were obtained from one continuous simulation run for 1973. The simulated runoff values (Figure 4) agree quite well with recorded data except for the spring period. The hydrology parameters were calibrated on 7.5 months of data in 1972; the calibration results were reported in the PTR Model report (1). Additional trial runs have indicated that the hydrologic characterisitcs appear to vary on a seasonal basis. During the dry summer- fall period, the watershed is highly responsive, producing short-duration sharp-peaked hydrographs from the thunderstorms that occur in the area. In the wetter winter-spring period, the watershed response is much more moderate with less erratic hydrographs extending over a longer duration. Since most pesticide loss occurs during the summer months, the simulation studies were concentrated on the critical summer.

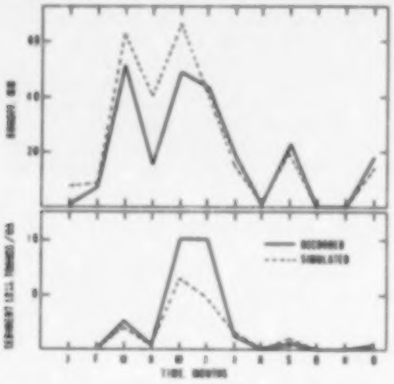


Figure 4 1973 monthly rainfall, runoff and sediment loss for the P1 watershed

The monthly sediment simulation in Figure 4 indicates the impact of tillage operations. Major storms occurred in May and June immediately following tillage of the watersheds. In fact, the recorded monthly sediment loss in May and June was estimated due to equipment malfunctions resulting from the high sediment load. Except for these two months, the simulated and recorded sediment loss are reasonably close. Since the sediment algorithms were modified during this study, the simulation shown in Figure 4 was obtained through calibration of the sediment parameters. More experience with the sediment algorithms on different watersheds is needed to truly verify the methodology.

The monthly pesticide simulation results are shown in Figure 5 for paraquat and diphenamid. The simulation values were obtained with parameters evaluated from laboratory data and the literature; calibration of pesticide parameters was minimized in order to evaluate the applicability of the algorithms using parameters from the literature. The agreement between the simulated and recorded monthly values is fair. The following points are indicated:

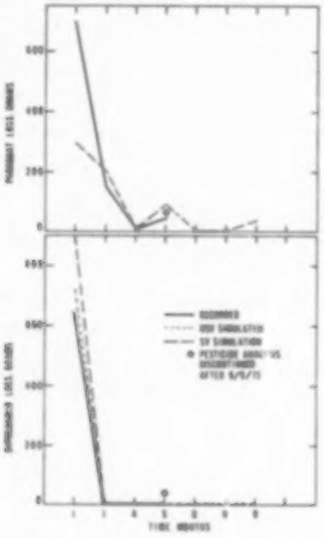


Figure 5 Monthly paraquat and diphenamid loss from the P1 watershed for the 1973 growing season

(1) Since paraquat is entirely (and essentially irreversibly) adsorbed onto sediment particles, pesticide loss closely parallels sediment loss. Both the recorded and simulated values demonstrate this behavior. Thus more accurate simulation of sediment loss would improve the paraquat simulation.

(2) Diphenamid is transported both in solution and on sediment particles; thus an initial comparison of the SV and NSV adsorption/desorption algorithms was possible. Although the diphenamid simulation in Figure 5 agrees well with the recorded values, results for various and other watersheds indicate that further investigation is warranted. The SV function performs better for some storms, while the NSV function performs better for others.

(3) The importance of attenuation processes is demonstrated by both the paraquat and diphenamid data. The large majority of pesticide loss occurs within one to two months following application (June 13, 1973 for the P1 watershed). Thus the first storm events immediately following application are the critical ones for pesticide transport from the land surface.

Numerous storm events were simulated during 1973. Figures 6 and 7 present the results for the storm of June 21, 1973. This storm occurred one week after planting and is one of the better simulated storms during the summer period. The original report (2) includes similar figures for various events to indicate the variability of the simulation results. The storm runoff and sediment loss for the June 21st storm is well simulated. The pesticide loss for both paraquat (Figure 6) and diphenamid (Figure 7) is plotted in terms of mass removal, i.e. pesticide mass per unit time. This representation demonstrates the close association between pesticide loss and the transport mechanisms of runoff and sediment loss. Although the SV function more closely represents the recorded diphenamid loss in Figure 7, as mentioned above the NSV function performed better for other storms. In essence, Figures 6 and 7 demonstrate the type of comparisons that must be made for storm events when analyzing the ability of a model to represent agricultural runoff.

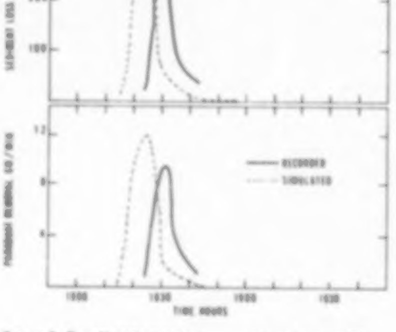


Figure 6 Runoff sediment and paraquat loss from the P1 watershed on June 21 1973

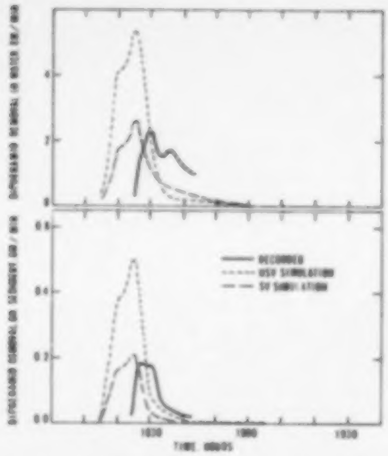


Figure 7 Diphenamid loss in water and on sediment from the P1 watershed on June 21 1973

Conclusions

The testing of the ARM Model has indicated that the hydrology and sediment simulations reasonably represent the observed data while the pesticide simulations can show considerable deviation from recorded values. This is especially true for pesticides that move by both runoff and sediment loss. The effects of tillage operations and management practices need to be further evaluated for hydrology and sediment production. Parameter changes as a result of agricultural practices need to be quantified. Although the results of sediment simulation have been promising, certain deviations in the results indicate a lack of understanding of certain aspects of the physical process. Other processes in the soil erosion mechanism, such as natural compaction of the surface following tillage and the effect of rainfall intensity on the transport capacity, need to be evaluated for possible inclusion in the Model. Although the hydrology model has been applied to hundreds of watersheds in the United States, the accompanying sediment model has been applied to only a few. If the ARM Model is to be generally applicable, the most immediate need is to evaluate the sediment simulation capability in varying climatic and edaphic regions.

For pesticide simulation, the results demonstrate the need to further investigate the processes of pesticide degradation and pesticide-soil interactions. Both the SV and NSV adsorption/desorption functions require further research. A non-equilibrium approach should be investigated to determine its applicability. The interactions in the active surface zone appear to control the major portion of pesticide loss especially for highly sediment-adsorbed pesticides like paraquat. The depth of the active surface zone and the extent of pesticide degradation in that zone are critical to the simulation of pesticide loss for any storm event. The need for testing the ARM Model in other regions also pertains to both the pesticide and nutrient functions. The processes recommended above for further research should be studied and evaluated in many regions of the country to determine the impact of soil and climatic conditions.

The final version of the ARM Model will be designed for use by state and local agencies across the country. This work has demonstrated that simulation models can be developed to represent the processes important to the quality of agricultural runoff. Moreover, continuous simulation models can be employed to develop probability distributions for sediment, pesticide, and nutrient loss as a basis for economic evaluation (15). In this way, models, like the ARM Model, can provide a valuable tool for planning and evaluation of pesticide regulations, fertilizer application, and other agricultural management practices.

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MODELING THE EFFECT OF PESTICIDE LOADING ON RIVERINE ECOSYSTEMS

J. W. Falco
Research Chemical Engineer
US Environmental Protection Agency
Environmental Research Laboratory
Athens, Georgia 30601

L. A. Mulkey
Agricultural Engineer
US Environmental Protection Agency
Environmental Research Laboratory
Athens, Georgia 30601

Abstract

A mathematical model for predicting the fate and transport of malathion in riverine ecosystems has been developed. The model predicts the concentration of malathion down the length of a river reach as a function of time and non-point source loading. Model simulations predict that standing crops of various fish species and other organisms decrease with increasing malathion concentration. Mass die-offs were predicted at critical malathion loadings and concentrations.

Introduction

Under Section 208 of Public Law 92-500, approximately 150 designated areas of the country will require area-wide waste treatment management plans. In light of a recent court test (National Resources Defense Council versus the US Environmental Protection Agency), many other areas will also require basin-wide plans. There are numerous problems which must be considered in area-wide planning. One can broadly classify these problems into two areas, evaluation of: (1) point source related problems, and (2) non-point source (NPS) related problems. Furthermore, NPS problems can be divided into urban and non-urban runoff related problems.

In evaluating potential water pollution impacts from non-point sources, mathematical models and statistical correlations provide a powerful analytical tool, particularly when limited data exist. These models provide the means to determine major potential NPS impacts; e.g., sediment loads created by agricultural practices in a given area. Secondly, these models provide the means to estimate the consequences of management decisions on a basin scale.

A number of models and correlations are available in the public domain for NPS pollution evaluation. For estimation of pollutant loads from single storm events, the "Storm Watershed Management Model (SWMM)," developed by Metcalf and Eddy, Inc.; University of Florida; and Water Resources Engineers, Inc., can be used.[1] For long-term pollutant loads based on annual average loadings, statistical correlations developed by McElroy et al. can be used.[2]

For continuous simulation of multiple storm events, two models are available. STORM is a runoff model developed by Water Resources Engineers, Inc., and revised by the US Army Corps of Engineers.[3] This model accounts for variation in surface water storage but does not account for water storage in subsurface compartments of watersheds. Consequently, it does not accurately simulate water movement in the watershed during dry periods between storm events. Both SWMM and STORM are particularly suited for and used extensively in analyzing urban NPS problems.

Hydrocomp Corporation has done a great deal of research on continuous simulation models which predict runoff continuously from multiple storm events. Unlike STORM, these models account for subsurface water movement, and are more comprehensive in terms of estimating water movement on the watershed between storm events. Two models which have recently been developed by Hydrocomp have potential application for basin-scale planning. The "Agricultural Runoff Model (ARM)"[4] is a continuous simulation runoff model which simulates pesticide and nutrient loads. In addition to simulating pesticide-soil interactions, the model also simulates soil nutrient transformations. The NPS Model[5] simulates pollutant contributions to streamchannels from both urban and non-urban sources. The model is keyed to the transport of sediments over the watershed. Potential basin applications include analysis of BOD-DO, temperature, and suspended solids related problems.

Similarly, there are a number of water quality models which can be used in non-point source pollution analysis. QUAL I,[6] QUAL II,[7] DOSAG,[8] and, to a lesser extent, AUTO-QUAL,[9] are river models which are applicable for analysis. It should be noted that most of these models require lumping of non-point sources into a small number of equivalent point sources. In addition, many variants of the previously referenced river models are also available. The most significant of these is the EXPLORE-I model.[10] In addition to the mass balance equations incorporated into the above mentioned models, EXPLORE-I also contains a momentum balance which permits flood routing during storm events.

This paper focuses on NPS problems associated with non-urban areas. Specifically, it deals with the impact on rivers of application of malathion, an organo-phosphorus pesticide, on agricultural watersheds. We have chosen this problem as a demonstrative example because it clearly illustrates the unique nature of non-point source problems and because a sufficient amount of data was available on this compound.

For evaluation purposes, ranges of malathion loads were inputted into a river quality model to show the effects on different species of fish. These loads were pulses in time along the entire length of the river section of interest. Eventually we intend to link ARM with the water quality model and simulate a series of storm events which were actually observed on experimental watersheds. Based on biological and chemical processes for which we have data, a time series of malathion concentration profiles down the length of the river reach were calculated and potential reduction in the standing crops of Carp, Striped Bass, and Bluegills were estimated.

Mathematical Development

The receiving water model used to predict the impact of malathion loads is a modification of a pesticide transport model developed by Falco et al.[11] It is essentially a material balance which accounts for the transport and transformation of chemical and biological constituents which are involved in the chemical and biological degradation processes. With one exception, the continuity equation used for each constituent is as follows:

$$\frac{\partial C_i}{\partial t} = D\frac{\partial^2 C_i}{\partial x^2} - v\frac{\partial C_i}{\partial x} + S_i \pm \sum_j R_{ij} \qquad (1)$$

where C_i = concentration of constituent i
D = dispersion coefficient
R_{ij} = rate of production or elimination of constituent i by pathway j
S_i = source strength of component i
t = time
x = distance in the direction of flow

This form of the continuity equation assumes that flow is one dimensional and that the cross-sectional area of the river reach is constant. We have assumed that, in the case of fish which are adversely affected by malathion, these organisms are stationary; i.e.,

$$\frac{\partial C_i}{\partial t} = -R_i \qquad (2)$$

where R = rate of reduction of the standing crop of organism i due to the presence of malathion

Equation 2 assumes that there is no net transport of organisms over the length of the stream. This is not a particularly realistic assumption. The reason we have used it is to clearly illustrate the deleterious effects of high malathion concentrations on a test set of organisms. It should be noted that this assumption eliminated the possibility of using this version of the model to predict natural restocking of fish by invasion from unaffected areas.

Two processes which are responsible for malathion degradation in aquatic ecosystems have been included in the model. The chemical degradation pathway modeled is alkaline hydrolysis. A detailed discussion of the chemical reactions involved in this pathway has been presented by Wolfe.[12] Wolfe's[12] results indicate two competing temperature dependent reactions occur. The first reaction, favored at low temperatures, results in the formation of an intermediate malathion monoacid product. An elimination reaction, favored at high temperatures, results in production of diethyl furmarate and O,O-dimethyl-phosphoro-dithioic acid.

In modeling these two reactions, we have assumed that the overall chemical degradation of malathion is a second order reaction; i.e.,

$$R_{hydrolysis} = -k_1 C_{OH} C_M \qquad (3)$$

where k_1 = second-order rate coefficient
C_{OH} = concentration of hydroxide ion
C_M = concentration of malathion

Since the two competing reactions have been combined, the rate constant k_1 is the sum of the individual rate constants for each of the competing reactions; i.e.,

$$k_1 = k_{elim} + k_{hydrol} \qquad (4)$$

Using the data provided,[12] the variation of these two rate coefficients can be fit to an exponential function,

$$k_{elim} = A_1 \exp\left[-\frac{A_2}{T}\right] \qquad (5)$$

$$k_{hydrol} = B_1 \exp\left[-\frac{B_2}{T}\right] \qquad (6)$$

At temperatures usually associated with natural environments, the hydrolosis reaction is favored. Thus, it was assumed in the model that chemical degradation of malathion and the appearance of α-malathion monoacid are stoichiometrically related. Consequently,

$$R_{\alpha\text{- monoacid}} = \gamma_1 k_1 C_{OH} C_M \qquad (7)$$

where γ_1 = yield of α- monoacid from malathion

For microbial degradation, Paris[13] proposed two models. The first used was the standard Monod expression for growth of organisms and limiting substrate utilization. The second model assumed second order reaction between malathion and bacteria. The standards of deviation calculated for least squares fits of the data to both models indicated that the second order reaction model gave the best fit. In the model constructed by Falco,[11] a Monod expression was used to approximate the growth of bacteria on a readily degradable carbon source, and a second order rate equation was used to describe the degradation of malathion by bacteria; i.e.,

$$R_{Bacteria} = \frac{\gamma \cdot \mu_{max}}{k_m + C_1} \cdot C_B \cdot C_1 - k_3 \cdot C_B \qquad (8)$$

$$R_{C_1} = -\frac{\mu_{max} \cdot C_1 \cdot C_B}{(K_m + C_1)} \qquad (9)$$

$$R_{mal} = -k_2 C_B C_M \qquad (10)$$

where $R_{Bacteria}$ = net rate of increase of bacteria
R_{mal} = microbial degradation rate of malathion
R_{C_1} = rate of carbon utilization
C_B = concentration of bacteria
C_1 = concentration of carbon source
μ_{max} = maximum growth rate of bacteria on specified carbon source
K_m = half-saturation constant for bacterial growth on specified carbon source
k_2 = specific microbial degradation rate for malathion
k = specific bacterial death rate
Y = bacteria growth yield

It should be noted that equation 8 includes a term, $k_3 C_B$, to account for the death of bacteria under starvation conditions.

Paris observed that the major product of bacterial mediated malathion degradation was β- malathion monoacid.[13] Consequently, malathion degradation and formation of β- monoacid are stoichiometrically related; i.e.,

$$R_{\beta\text{- monoacid}} = \gamma_2 k_2 \cdot C_3 \cdot C_M \qquad (11)$$

where γ_2 = yield of β- monoacid from malathion

In this paper, the bacterial degradation model used is the one developed by Falco.[11]

To summarize briefly, the water quality model used accounts for transport of chemical constituents: malathion, α- monoacid, β- monoacid, and degradable carbon and bacteria by equation 1. The degradation of malathion which appears as a sink term $(\sum_j R_{ij})$ in equation 1 is accounted for by equations 3 and 5. The growth and death of bacteria are accounted for in the transport equation for bacteria by inclusion of equation 8. The uptake of degradable carbon is accounted for in its transport equation by substitution of equation 9 for $(\sum_j R_{ij})$ in equation 1. The source terms in the equations which describe the transport of α- and β- monoacids are defined by equations 7 and 11, respectively. Lastly, the toxic effects of malathion on standing crops of fish are modeled according to equation 2, where it is also assumed that

$$R_i = -k_4 C_M C_F \qquad (12)$$

and C_F = concentration of organisms effected by malathion
k_4 = specific death rate

The only required relationships which we have not discussed are the boundary and initial conditions which are applicable to the river system. These, along with a description of the nature of the sources of pollutant loads (S_i) are specific to the particular problem being investigated.

Results and Discussion

The equations discussed in the previous section were coded into a Fortran program described by Falco.[11] The appropriate coefficients used for each simulation are listed in Table 1.

μ_{max} (mg org^{-1} hr^{-1})	k_m (mg $ℓ^{-1}$)	k_1 (M^{-1} hr^{-1})
7.2×10^{-10}	6.3	1.43×10^4

k_2 (ℓ org^{-1} hr^{-1})	k_3 (hr^{-1})	γ_1 (mg/mg)
1.21×10^{-12}	5.16×10^{-3}	0.915

γ_2 (mg/mg)	Y (org/mg)
0.915	5.73×10^9

Table 1. VALUES OF RATE COEFFICIENTS AND YIELD FACTORS USED IN ALL SIMULATIONS.

For all simulations shown, it was assumed that a significant point source of readily available carbon was located 16 km from the upstream reference point with a discharge rate of 10.9 kg/day of usable carbon. For simulations in which reduction in fish populations were projected, it was assumed that malathion degraded via alkaline hydrolysis at a rate which would correspond to a pH 8. This is an extremely high pH which is not very likely to occur in streams. We have used it here because it predicts a rapid decay in malathion. As it will be shown, in spite of this rapid decay, standing crops of fish are severely affected under moderate malathion loads. The point is, even under the most favorable conditions for malathion degradation, material entering the system can be present long enough to have an adverse impact.

The physical characteristics of the system we have simulated are shown in Table 2.

River cross-sectional area	River length	Surface area of basin	Average river velocity
30 m^2	129 km	25.8 km^2	9 m/min

Table 2. PHYSICAL CHARACTERISTICS OF THE SYSTEM.

For simulations in which fish population reductions were projected, the following specific death rates were used:

1. For Carp, $k_4 = 1.44 \times 10^{-3}$ ℓ mg^{-1} hr^{-1}
2. For Striped Bass, $k_4 = 3.28 \times 10^{-2}$ ℓ mg^{-1} hr^{-1}
3. For Bluegill, $k_4 = 0.135$ ℓ mg^{-1} hr^{-1}

These values were obtained by fitting toxicity data for 24, 48, and 96 hr TL_m concentrations reported by Ferguson[14] to an exponential function in malathion concentration and time; i.e.,

$$0.5 = \exp\left[-k_{*} \cdot C_{TL_m} \cdot t_{TL_m}\right] \qquad (13)$$

where t_{TL_m} = exposure time

C_{TL_m} = measured toxicity of malathion

Figure 1 shows the steady state concentration profile which would exist if the loading rate for malathion were 0.126 gm/acre day. The contribution of microbial and chemical degradation are also shown along with the concentration profile that would exist if neither of these two processes occurred. Under the conditions simulated, both alkaline hydrolysis and microbial degradation are important processes for the elimination of malathion.

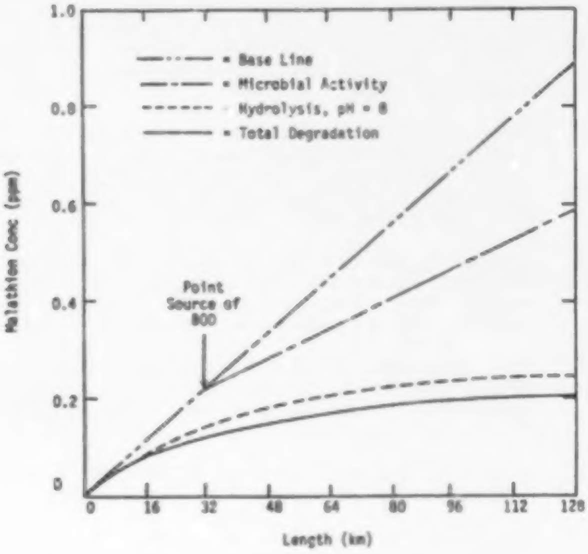

Figure 1. Comparison of steady-state malathion concentration profiles in response to a load of 0.126 gm/acre day.

Figures 2 and 3 show the response of the river to a pulse of malathion loaded over a period of two days in the amount of 700 mg/acre. Figure 2 shows the concentration profiles for malathion as the pesticide is degraded and diluted out of the river. Figure 3 shows the concentration profiles of α- malathion monoacid as it is formed and diluted out of the river. Comparing the two graphs, it can be seen that the monoacid persists in the river for longer periods of time than malathion. Because of its relative persistence, more information is needed on this degradation product.

Figures 4 and 5 show the relative standing crops of Carp, Bass and Bluegill before and after a storm event in which malathion is loaded into the river. Figure 4 shows the impact of runoff amounting to 700 mg/acre and Figure 5 shows the impact of runoff loads were chosen to demonstrate the variation in species response to a range of malathion inputs. Based upon recommended application rates of malathion, the range of loads used in these examples are possible. However, neither field data nor simulation loading model results are available to determine the probability of occurence of such loads or to delineate the actual physical conditions under which they may occur. The projections indicate that severe damage could occur to both Bass and Bluegill at the higher loading. At low loading rates, only Bluegills are adversely affected.

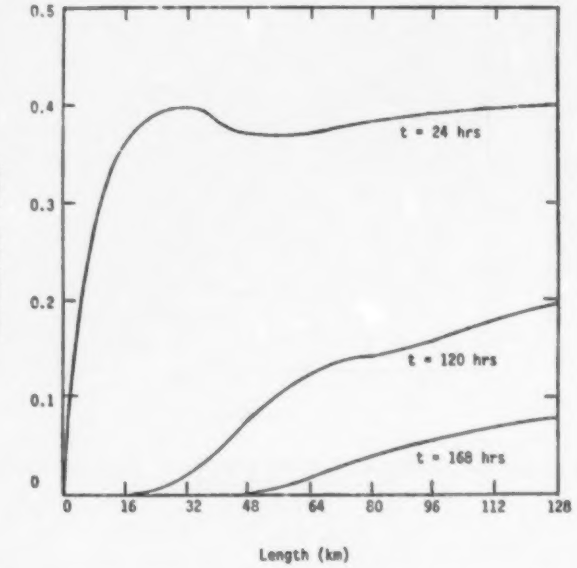

Figure 2. Response of a stream to a pulse of malathion of 700 mg/acre.

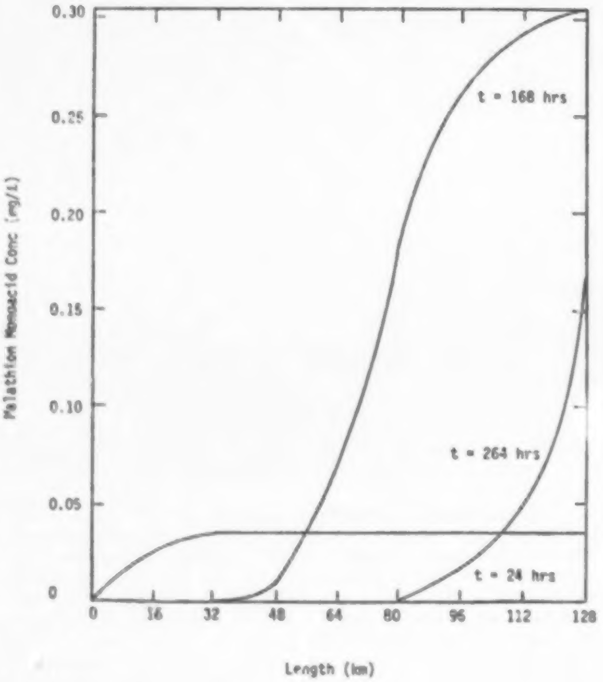

Figure 3. Concentration profiles of α- malathion monoacid as a function of time in response to a 700 mg/acre pulse of malathion.

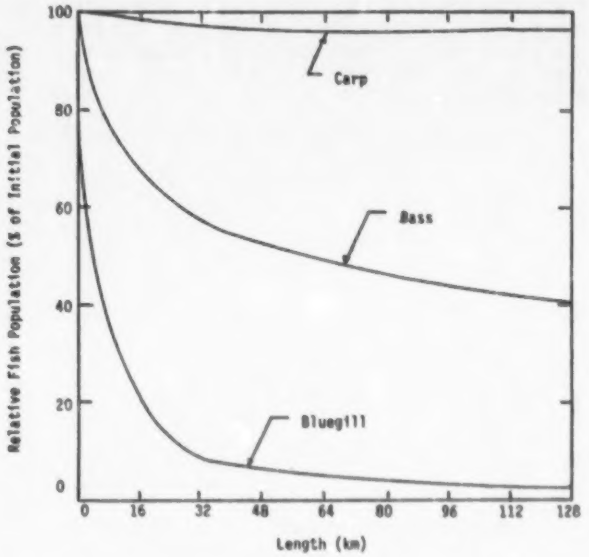

Figure 4. Response of three species of fish to a pulse of malathion of 700 mg/acre.

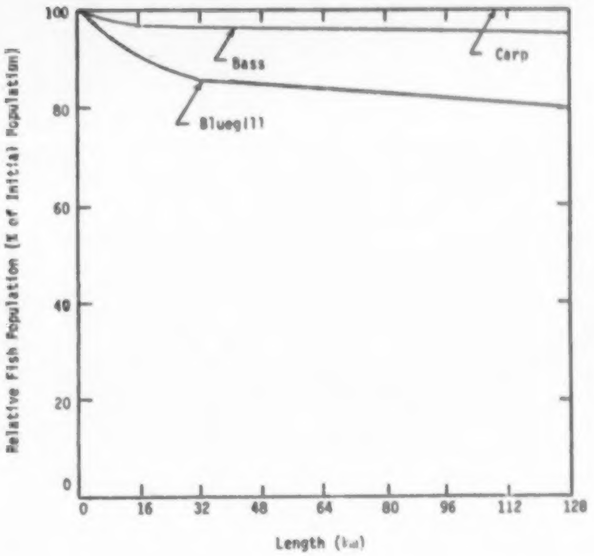

Figure 5. Response of three species of fish to a pulse of malathion of 44 mg/acre.

In summary, we have presented an analysis and projected the impact of a pesticide on three species of fish. We have indicated the types of information necessary for this analysis. Although the absolute values of coefficients and parameters may vary from one problem to another, the procedure should be applicable to many situations. The use of this model and eventually more sophisticated ones as they are published should provide insight into a broad range of NPS pollution problems.

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RADIONUCLIDE TRANSPORT IN THE GREAT LAKES

R. E. Sullivan, Ph.D.
Environmental Protection Agency
Office of Radiation Programs
Washington, D. C.

W. H. Ellett, Ph.D.
Environmental Protection Agency
Office of Radiation Programs
Washington, D. C.

Summary

A mathematical model has been developed to predict radionuclide levels in the Great Lakes due to nuclear power generation in the United States and Canada. The calculations have been used to verify the feasibility of proposed International water quality objectives for radioactivity in the Lakes. Dose rates and doses to reference-man from the ingestion of Lake waters are predicted based on expected future power generation in this region.

Introduction

A recent bipartite agreement between the United States and Canada on water quality in the Great Lakes mandated establishment of a radioactivity objective for the Lakes. The liquid effluents discharged into the Great Lakes from nuclear power plants and other nuclear facilities, such as fuel reprocessing plants, are of particular interest in this regard since some of the entrained radionuclides have relatively long half-lives.

Previous work in this area [1,2] has been concerned mainly with fallout from nuclear weapons tests. Since in this study we are primarily concerned with predicting the concentrations of specific radionuclides emitted in the nuclear fuel cycle and the resultant doses to reference-man, the contribution from fallout has been neglected. However, such source terms may be included by specifying appropriate initial concentrations for these radionuclides.

A simplified model of the Great Lakes system has been employed which assumes perfect mixing but allows for the periodic establishment of a thermocline by varying the mixing volume. Corrections are made, where necessary, for removal of radionuclides by sedimentation and equilibration. The results are given in terms of radionuclide concentrations in each lake and the dose rates and doses ensuing from continuous, long-term ingestion of system waters. With the model described, it is possible to obtain analytical solutions for the coupled differential equations describing these quantities as a function of time. However, a FORTRAN computer program has been employed to reduce the calculational effort required.

In succeeding sections, we present a description of the physical and mathematical models developed, the rationale employed in specifying source terms for various types of facilities, and details of the dose calculation. A sample problem, projecting the future effects of radioactive contamination of the Great Lakes due to projected nuclear plant operations, is described in some detail. Results from this and similar problems have been used to verify the feasibility of the water quality objectives set by the U.S.-Canada agreement.

Physical Model Analysis

Radionuclide Concentrations

The physical model of the Great Lakes comprises a set of five bodies of water characterized by constant total volume, inflow, outflow, and surface area. The lakes are interconnected so that, with the exception of Lakes Superior and Michigan, each may contribute radioactivity to succeeding members of the chain as indicated in Figure 1.

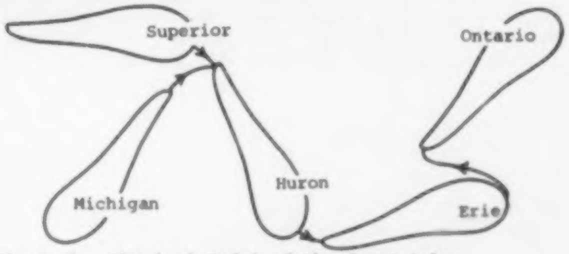

Figure 1. Physical Model of the Great Lakes

The governing differential equation for models of this type, for the ith lake and a single nuclide is:

$$V_i \frac{dC_i}{dt} = R_i - \lambda_r C_i - \lambda_p C_i - q_i C_i + \sum_{j<i}^{i>2} q_j C_j \qquad (1)$$

where

C_i = concentration for ith lake [Ci/cm^3]

R_i = input rate into ith lake [Ci/yr]

V_i = mixing volume of ith lake [cm^3]

λ_r = radioactive decay constant for this nuclide

λ_p = decay constant for physical removal (sedimentation, equilibration) [yr^{-1}]

q_i = volumetric flow out of ith lake [cm^3/yr]

Because of the summation on j, a major difficulty in solving the equation arises in that each C_j term embodies the complete differential equation for all preceeding lakes, thus complicating the expressions for the lower lakes.

We have chosen to apply the Laplace transform in order to obtain solutions to these equations. the transformed equation for C_i is

$$c_i(s) = \frac{R_i}{V_i}\left[\frac{1}{s(s+k_i)}\right] + \frac{C_i^0}{(s+k_i)} + \sum_{j<i}^{i>2} \frac{q_j c_j(s)}{V_i(s+k_i)} \tag{2}$$

where $k_i = (\lambda_r + \lambda_p + \frac{q_o}{V})$ depends on both the characteristics of the lake (i) and the physical properties of the radionuclide. C_i^0 is the initial lake concentration. For Lakes Superior and Michigan, which have no lake tributaries, the C_j term vanishes and the equation (2) reduces to

$$c_i(s) = \frac{R_i}{V_i}\left[\frac{1}{s(s+k_i)}\right] + \frac{C_i^0}{(s+k_i)} \tag{3}$$

The general equation becomes increasingly more complex as we proceed down the chain of lakes. However, the transformed solutions to these general equations comprise only terms of the form

$$c(s) = \frac{f(s)}{g(s)}$$

in which f(s) is constant and g(s) is the product of linear, non-repeated factors,

$$g(s) = (s+k_1)(s+k_2)\cdots(s+k_i) \tag{4}$$

To reduce the effort required in solving such expressions, a variation of Heavisides' partial fraction expansion[3],

$$L^{-1}\left\{\frac{1}{g(s)}\right\} = \sum_{n=1}^{i} \frac{1}{g(k_n)} e^{-k_n t} \tag{5}$$

is applied. Here, $g(k_n)$ denotes the product of all the factors except the factor $(s-k_n)$. Using (5), the solution to equation (3) for Lake Michigan or Lake Superior is

$$C_i(t) = \frac{R_i}{V_i}\left[\frac{1}{k_i} - \frac{1}{k_i} e^{-k_i t}\right] + C_i^0 e^{-k_i t} \tag{6}$$

For the next lake (Huron) equation (2) includes expressions for the preceeding lakes

$$c_i(s) = \frac{R_i}{V_i}\left[\frac{1}{s(s+k_i)}\right] + \frac{C_i^0}{(s+k_i)} + \tag{7}$$

$$\left\{\sum_{j=1}^{2} \frac{q_i}{V_i}\left[\frac{1}{(s+k_i)}\right] \frac{R_j}{V_j}\left[\frac{1}{s(s+k_j)}\right] + \frac{C_j^0}{(s+k_j)}\right\}$$

where the summation over j indicates the presence of two terms, one for Lake Superior and the other for Lake Michigan, the c(s) terms for these lakes corresponding to the $c_j(s)$ terms in equation (2).

It is evident that as the differential equation for each lake in the progression is transformed, each term will contain an additional factor (s + k) Again, solutions are found by means of the inverse transform of equation (5), which yields the concentration of a specified radionuclide as a function of time.

Dose Rate and Dose to Reference-Man

The concentrations of radioactivity in lake water can be used to find the annual dose rate due to ingestion of lake water by reference-man. Because the radioactivity in the lakes is expected to be a strongly varying function of time, due to the rapid projected growth of nuclear power, dose estimates cannot be based on a constant intake of activity over the time necessary to reach equilibirum in the body except for nuclides having a relatively short effective half-life. Nor can the dose over a 50-year period be determined using the conventional models given in ICRP Publication 2.[4] Rather, in this study the dose rate and dose calculations are based on equations and data presented in ICRP 10[5] and ICRP 10A[6]. However, for organ burden, b(t), and cumulated activity , B(T), the equations have been revised slightly to conform to program usage. Both dose and dose rate are predicated, at present, solely on an assumed consumption by reference - man of 2.2 liters of drinking water per day. This quantity is somewhat larger than that usually consumed as drinking water to account for the contribution to the body burden from food pathways.

Over a time interval short enough to allow treating the average concentration as constant, the intake, I(t), is directly proportional to the lake concentration. Integration of the ICRP equations for organ burden and cumulated activity are straightforward if the retention function, R(t), contains only exponential terms. For the isotopes of interest here retention functions of this form are given in reference 5. For ingestion at a constant average intake, I,

$$b(t) = I \int_0^t R(t-\tau)\, d\tau \tag{8}$$

and

$$B(T) = \int_0^T \int_0^t R(t-\tau)\, d\tau\, dt \tag{9}$$

Since the retention function, R(t), is the sum of a series of exponentials,

$$R(t) = \sum_{n=1}^{N} \alpha_n e^{-\beta_n t} \tag{10}$$

each term in the integral defining the organ burden will be of the form

$$b_n(t) = I\int_0^t a_n\, e^{-\lambda_n(t-\tau)}\, d\tau \tag{11}$$

There are two solutions for this equation. The first yields the organ burden

$$b_n(t) = \frac{a_n I}{\lambda_n}\left[1 - e^{-\lambda_n(t-t_1)}\right] \tag{12}$$

at any time during the period, beginning at time t_1, of ingestion. The second solution gives the organ burden at any time subsequent to t_2, the end of the ingestion period.

$$b_n(t) = \frac{a_n I}{\lambda_n}\left[e^{-\lambda_n(t-t_2)} - e^{-\lambda_n(t-t_1)}\right] \tag{13}$$

The instantaneous dose rate depends only on the organ content at some time t. However, cumulated activity and, therefore, the dose depend on the whole time history of ingestion so that the sum of equations (12) and (13) must be used in evaluation of the total dose over a period T. The cumulated activity is then

$$B_n(T) = a_n I\left\{\int_{T_1}^{T_2}\left[1 - e^{-\lambda_n(t-t_1)}\right]dt + \int_{T_2}^{T}\left[e^{-\lambda_n(t-t_2)} - e^{-\lambda_n(t-t_1)}\right]dt\right\} \tag{14}$$

where T_1, T_2, and T are analogous to the t values used in the organ burden equations. Performing the integration and collecting terms,

$$B_n(T) = \frac{a_n I}{\lambda_n}\left\{(T_2-T_1)+\frac{1}{\lambda_n}\left[e^{-\lambda_n(T-T_1)}-e^{-\lambda_n(T-T_2)}\right]\right\} \tag{15}$$

with a similar term for each exponential needed in the retention function. Note that, since intake is directly proportional to lake concentration (which comprises only constant and exponential terms), equations (8) and (9) may be solved analytically. However, for the short time intervals considered here (one year) the use of an average I is sufficient.

Computer Program Analysis

The basic program uses three loops to account for the dependence on time, lake and isotope. The time loop is usually solved in one-year increments and, to account for the existence of a thermocline, mixing during the first half year is based on the total lake volume while in the last half year a 17-meter depth (thermocline) is presumed and the product of this depth and the lake surface area define the mixing volume. The model assumes that lake outflows remain constant in the epilimnion, with equilibration dependent on the concentration above the thermocline. Nuclides in the hypolimnion are assumed to be removed only by radioactive decay and, where applicable, sedimentation.

Several options are available for defining the source terms, B. Specification of reactor type is required since the liquid discharges vary significantly between the various (BWR, PWR) types. These releases also depend on the sophistication of the liquid radwaste system employed by each type of reactor. Since detailed examination of the radwaste system for each operating reactor may not be practical and is not possible for plants scheduled for future operation, it has been necessary to make some assumptions regarding these releases. We have utilized the results of an in-depth environmental analysis[7] which presented typical releases expected from four classes each of BWR and PWR liquid waste system representing a range of treatment from minimum to maximum. This data is incorporated into the computer program for use in a source input option. Thus, the simplest input consists of specifying the number of BWRs and PWRs (nominal 1000 MWe) on each lake along with the appropriate choice of radwaste system type (1 through 4) and allowing the program to internally generate source terms for each lake and isotope. Alternatively, the actual source terms for each lake and isotope may be directly entered or the two options may be combined.

The data required to obtain solutions for five isotopes (H^3, Co^{60}, Sr^{90}, Cs^{134}, Cs^{137}) is presently stored in the program, but other radionuclides may easily be added. At present, this data includes correction factors, in the form of the effective decay constants indicated in equation (2), to account for equilibration of tritium[8] and sedimentation of cesium[9].

The standard output consists, for each isotope, of the average radionuclide concentrations for each year and Great Lake. A summary table giving annual dose rates and cummulative doses by year for each lake is also printed out. The critical organ assumed for each isotope is identified at the head of each column.

Problem Description

The underlying purpose of this analysis and the resulting computer program was to estimate the effect on the Great Lakes of nuclear power plant operation through the year 2050. These estimates were needed in order to establish reasonable estimates of water quality for the lakes. To obtain a valid assessment it is necessary to consider not only the effluent from the plants themselves, but also that from any reprocessing plants located on the lakes. Separate determinations were made for each of the sources described below in order to compare the relative effects of each.

Sources

U.S. Nuclear Power Stations

The total number of nuclear power plants in the United States has been estimated by interpolation of data contained in a compilation issued by the AEC.[10] The apportionment of reactors to the Great Lakes basin and to the individual lakes was taken to have the same ratio to the total number as the known 1980 values.

U.S. Fuel Reprocessing Plants

Only one reprocessing operation, the Nuclear

Fuel Services plant, is presently scheduled for the Great Lakes basin. The source terms for this facility were taken from the associated Environmental Impact Statement.[11] One additional facility, located inland but contributing to the tritium concentration in Lake Michigan by rainout, has been postulated.

Canadian Power Stations

Source terms for the Canadian heavy water reactors expected to be in use during this period have been estimated from current data furnished by facility operators.[12] It should be noted that these values are very conservative and may overestimate the activity entering the Lakes from Canadian reactors. In particular, tritium discharges are expected to be reduced in the future due to the economic incentive to conserve heavy water.

Results

Using the general procedure described in the text, the nuclide concentrations, dose rates, and cumulative doses have been determined for the period 1962-2050. Two sets of operating conditions have been used: in the first, the nuclear facilities operating in the year 2000 have been assumed to continue operation at a constant level until 2050. In the second, all sources have been presumed to be removed after the year 2000 in order to estimate the time required for radioactive decay and lake turnover to clear the lakes. The only operational reactors in the period 1969-1970 were on Lake Michigan. Nuclide concentrations in the remaining lakes during this period are due to flow from Michigan through connecting rivers. Subsequent to this period, generating stations begin to come on line in the other lakes until, by 1980, operating reactors are projected for all lakes but Superior. Lakes Erie and Ontario, which not only have large numbers of facilities but receive the effluent from other lakes, have roughly twice the nuclide concentrations of the other lakes. Radioactivity concentrations are rather insignificant until after 1980 when there is a sharp rise through the year 2000.

To indicate the overall effect of nuclear power generation on radionuclide levels in the Great Lakes, the dose rates from each isotope considered are given in Table 1 for each lake. Table 2 shows the cumulative doses, by lake, incurred from ingestion of each nuclide through the year 2050. Both sets of results are for operation at a constant level through the year 2050 assuming the number of installations is constant after the year 2000.

Based on the model described in the text, by far the largest cumulative dose is due to the concentration of tritium in Lake waters. The vast majority of the tritium present is from fuel reprocessing activities and is in the effluent from Canadian heavy water reactors. However, the maximum seventy-year dose — from about 1980 to 2050 — is only 23 millirem, due to ingestion of Lake Ontario water. The remaining isotopes contribute less than 1 millirem to the total dose.

It should be noted that the results presented may be altered when refinements to the model (i.e., hydrographics, source, equilibration, sedimentation, etc.) are possible. In particular, the effects of localized near-shore currents may variably affect the concentration of isotopes in the drinking water intakes of cities adjacent to effluent discharges. On a long-term basis, however, in which relatively perfect mixing may be assumed, these results should not be affected drastically. Moreover, these results indicate that nuclide concentrations arising from currently projected nuclear fuel cycle operations yield radiation doses which lie within the proposed objective for Great Lakes Water Quality.

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TABLE 1

DOSE EQUIVALENT RATE IN THE YEAR 2050*
(microrem/year)

Isotope and Critical Organ		Lake Michigan	Lake Huron	Lake Erie	Lake Ontario
Tritium (Body Water)	1	6.402	5.205	13.36	11.34
	2			55.92	110.8
	3	55.38	22.48	15.91	8.797
	4		137.8	97.91	257.7
Cobalt-60 (Total Body)	1	0.007	0.004	0.017	0.012
	2				
	3				
	4		0.041	0.328	0.082
Strontium-90 (Bone)	1	2.633	2.434	5.189	5.121
	2			4.865	10.71
	3				
	4				
Cesium-134 (Total Body)	1	0.635	0.283	2.097	0.874
	2			0.176	0.195
	3				
	4		0.199	0.064	0.447
Cesium-137 (Total Body)	1	0.995	0.478	2.842	1.452
	2			0.140	0.178
	3				
	4		0.907	0.393	1.956

*After 50 years operation at constant source level.

1. U. S. Nuclear Power Reactors
2. NFS Fuel Reprocessing Plant
3. Postulated H-3 Rainout into Lake Michigan
4. Canadian Power Reactors

TABLE 2

DOSE EQUIVALENT BY THE YEAR 2050*
(microrem)

Isotope and Critical Organ		Lake Michigan	Lake Huron	Lake Erie	Lake Ontario
Tritium (Body Water)	1	332.0	247.9	727.5	584.1
	2			3852.0	7245.4
	3	2791.7	954.5	644.7	317.4
	4		7646.5	5236.5	14464.5
Cobalt-60 (Total Body)	1	0.372	0.226	0.998	0.691
	2				
	3				
	4		2.39	1.55	4.76
Strontium-90 (Bone)	1	100.6	79.89	218.7	209.6
	2		279.3	565.0	
	3				
	4				
Cesium-134 (Total Body)	1	40.06	16.66	124.3	51.76
	2			12.27	13.53
	3				
	4		12.42	3.93	27.59
Cesium-137 (Total Body)	1	61.81	27.74	167.2	84.43
	2			9.723	12.21
	3				
	4		55.74	23.69	119.02

*After 50 years operation at constant source level. lifetime dose.

1. Nuclear Power Stations
2. NFS Reprocessing Plant
3. Postulated H-3 Rainout into Lake Michigan
4. Canadian Power Stations

FEDBAK03 - A COMPUTER PROGRAM FOR THE MODELLING OF FIRST ORDER CONSECUTIVE REACTIONS WITH FEEDBACK UNDER A STEADY STATE MULTIDIMENSIONAL NATURAL AQUATIC SYSTEM

George A. Nossa
Environmental Engineer
Data Systems Branch
U.S. Environmental Protection Agency
New York, N.Y.

ABSTRACT

The computer model described is used to compute the steady-state distribution of water quality variables undergoing consecutive reactions with feedback and following first order kinetics. The program has been developed in a general form but is specifically applicable to the reactions observed by nitrogenous species and the associated dissolved oxygen uptake in the natural environment.

The basis for this model is the theory of conservation of mass. The approach used to solve the equations is a finite difference scheme developed by Thomann (4,5), which has been shown to be a very effective tool in the field of water quality management.

INTRODUCTION

A computer model has been developed to serve as a useful tool in the prediction of water quality parameters which react under first order kinetics and as a system of consecutive reactions,where any parameter can react in a feedback fashion. The problem setting assumes an aquatic environment in which steady state conditions can be applied

Lets consider a system of five reactants:

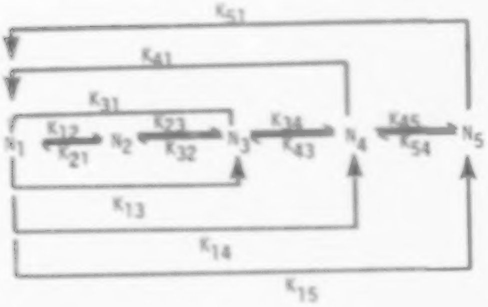

FIGURE 1
SCHEMATIC OF FIVE REACTANT SYSTEM

In the above system, the consecutive feedfoward and feedback reaction rates are presented. All the possible reaction loops for the first reactant have also been included. This particular system will be used in the theory development.

THEORY

The general estuarine advection/dispersion equation may be written as:

$$\frac{\partial N}{\partial t} = \frac{E\partial^2 N}{\partial x^2} - \frac{U\partial N}{\partial x} - KN + W_N(x) \ldots\ldots\ldots\ldots (1)$$

where:

N = concentration of constituent
t = time, in tidal cycles
E = tidally averaged dispersion coefficient which includes the dispersive effects of tidal motion
U = net advective velocity
K = first order decay coefficient of constituent N
W(x) = direct discharges of N

Assuming steady state conditions: dN/dt = 0 and equation (1) becomes:

$$0 = E\,\frac{d^2N}{dx^2} - U\,\frac{dN}{dx} - KN + W(x) \ldots\ldots\ldots\ldots (2)$$

Direct solutions for the above equation have been computed by O'Connor (1,2), a computer program has been documented by EPA, Region II (3) which uses this technique to solve for water quality parameters.

A second solution approach developed by Thomann (4,5) solves the above differential equation directly by replacing the derivatives with finite-difference approximations. This approach is used by computer program HAR03; documented by EPA, Region II (6) to analyze systems of consecutive reactions. The Thomann solution technique will also be the approach followed in program FEDBAK03.

If we take the first reactant N_1 on figure 1 and we incorporate all the feedback loops, equation (2) becomes:

$$0 = E\,\frac{d^2N_1}{dx^2} - U\,\frac{dN_1}{dx} - K_{11}N_1 + K_{21}N_2 + K_{31}N_3 + K_{41}N_4 + K_{51}N_5 + W_1 \ldots\ldots\ldots (3)$$

where K_{ij} are the appropriate first order reaction rate constants. The incorporation of the reaction term K_{11} allows for the first order decay of this first component out of the system.

For the other remaining reactants equation (2) would be written as:

$$0 = E\,\frac{d^2N_2}{dx^2} - U\,\frac{dN_2}{dx} - K_{22}N_2 + K_{12}N_2 + K_{32}N_3 + K_{42}N_4 + K_{52}N_5 + W_2 \ldots\ldots\ldots (4)$$

$$0 = E\,\frac{d^2N_3}{dx^2} - U\,\frac{dN_3}{dx} - K_{33}N_3 + K_{13}N_1 + K_{23}N_2 + K_{43}N_4 + K_{53}N_5 + W_3 \ldots\ldots\ldots (5)$$

$$0 = E\frac{d^2N_4}{dx^2} - U\frac{dN_4}{dx} - K_{44}N_4+K_{14}N_1+K_{24}N_2+K_{34}N_3+K_{54}N_5+W_4 \tag{6}$$

$$0 = E\frac{d^2N_5}{dx^2} - U\frac{dN_5}{dx} - K_{55}N_5+K_{15}N_1+K_{25}N_2+K_{35}N_3+K_{45}N_4+W_5 \tag{7}$$

The Thomann solution approach divides the system into completely mixed segments, as illustrated for a one dimensional estuary in figure 2.

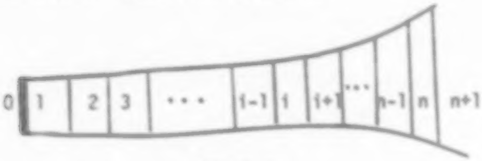

FIGURE 2
SEGMENTED ONE DIMENSIONAL ESTUARY

where segments 1 and 'n' each form an interface with the boundaries. Equation (3) for the "i" segment on figure (2) can be written as:

$$E_iA_il_i\frac{d^2N_{1,i}}{dx^2} - Q_il_i\frac{dN_{1,i}}{dx} - V_iK_{11,i}N_{1,i}+V_iK_{21,i}N_{2,i} + V_iK_{31,i}N_3+V_iK_{41,i}N_4+V_iK_{51i}N_5+W_1=0 \tag{8}$$

The derivatives on the equation above can be replaced by finite-difference approximations giving:

$$E_iA_il_i\frac{d^2N_{1,i}}{dx^2} = E'_{i-1,i}(N_{1,i-1}-N_{1-i})+E'_{i,i+1}(N_{1,i+1}-N_{1,i}) \tag{9A}$$

$$Q_il_i\frac{dN_{1,i}}{dx} = Q_{i,i+1}(\alpha_{i,i+1}N_{1,i}+\beta_{i,i+1}N_{1,i+1}) - Q_{i-1,i}(\alpha_{i-1,i}N_{1,i-1}+\beta_{i-1,i}N_{1,i}) \tag{9B}$$

where: $$E'_{i,j} = \frac{E_{i,j}A_{i,j}}{\bar{l}_{i,j}} \tag{9C}$$

i,j = subscripts used to denote the interface between adjacent segments i and j

$\bar{l}_{i,j}$ = average length of segments i and j = $(l_i+l_j/2)$

$\alpha_{i,j}$ and $\beta_{i,j}$ are weight factors to correct the concentrations from equation 9B

$$\alpha_{i,j} = \frac{l_j}{l_i+l_j} \tag{10}$$

$$\beta_{i,j} = 1 - \alpha_{i,j} = \frac{l_i}{l_i+l_j} \tag{11}$$

In order for the final concentrations to be positive, it is required that:

$$\alpha_{i,j} > 1 - E'_{i,j}/Q_{i,j} \tag{12}$$

Substituting equations (9A) and (9B) into equation (8) yields:

$$\begin{aligned}&E'_{i-1,i}(N_{1,i-1}-N_{1,i})+E'_{i,i+1}(N_{1,i+1}-N_{1,i})\\&-Q_{i,i+1}(\alpha_{i,i+1}N_{1,i}+\beta_{i,i+1}N_{1,i+1})\\&+Q_{i-1,i}(\alpha_{i-1,i}N_{1,i-1}+\beta_{i-1,i}N_{1,i})-V_iK_{11,i}N_{1,i}\\&+V_iK_{21,i}N_{2,i}+V_iK_{31,i}N_{3,i}+V_iK_{41,i}+V_iK_{51,i}\\&\qquad N_{5,i}+W_{1,i}=0\end{aligned} \tag{13}$$

Grouping terms in the above equation yields:

$$\begin{aligned}&(-Q_{i-1,i}\alpha_{i-1,i}-E'_{i-1,i})N_{1,i-1}\\&+(Q_{i,i+1}\alpha_{i,i+1}-Q_{i-1,i}\beta_{i-1,i}+E'_{i-1,i}+E'_{i,i+1}+\\&\qquad V_iK_{11,i})N_{1,i}\\&+(Q_{i,i+1}\beta_{i,i+1}-E'_{i,i+1})N_{1,i+1}=W_{1,i}+V_iK_{21,i}N_{2,i}\\&+V_iK_{31,i}N_3+V_iK_{41,i}N_4+V_iK_{51,i}N_5\end{aligned} \tag{14}$$

Letting:

$$a_{i,i-1}=-Q_{i-1,i}\alpha_{i-1,i}-E'_{i-1,i} \tag{15}$$

$$a_{i,i}=Q_{i,i+1}\alpha_{i,i+1}-Q_{i-1,i}\beta_{i-1,i}+E'_{i-1,i}+E'_{i,i+1}+V_iK_{11,i} \tag{16}$$

$$a_{i,i+1}=Q_{i,i+1}\beta_{i,i+1}-E'_{i,i+1} \tag{17}$$

The general equation for the ith segment becomes:

$$a_{i,i-1}N_{1,i-1}+a_{i,i}N_{1,i}+a_{i,i+1}N_{1,i+1}=W_{1,i}+V_iK_{21,i}N_{2,i}+V_iK_{31,i}N_3+V_iK_{41,i}N_4+V_iK_{51,i}N_5 \tag{18}$$

The use of this finite difference approximation scheme has a numerical dispersion, which can be approximated as (5)

$$E_{num} = U\bar{l}\,(\alpha-1/2) \tag{18A}$$

Where E_{num} is the numerical dispersion. This is particularly important to stream applications where advective velocities may be high and this effect may lead to distorted results.

Extension to multi-dimensional analysis:

If we consider a grid of orthogonally straped sections such as the one illustrated in figure 3:

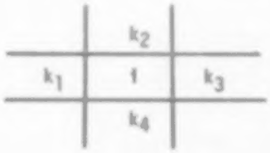

FIGURE 3
HYPOTHETICAL TWO DIMENSIONAL SYSTEM

Following the convention that flows entering a section is negative and flow out of a section is positive, a mass balance due to the transport and dispersion of material from section i to all surrounding sections k(s) is:(4,5,8)

$$V_i\frac{dN_{1,i}}{dt}=0=\sum_k -Q_{ik}(\alpha_{ik}N_{1,i}+\beta_{ik}N_{1,k})+E'_{ik}(N_{1,k}-N_{1,i})-V_iK_{11,i}N_{1,i}+V_iK_{21,i}N_{2,i}+\dots+V_iK_{51,i}N_{5,i}+W_{1,i}\quad (i=1,2\dots n) \tag{19}$$

This equation is the equivalent to equation (13) for the one dimensional case. The generalization of the advection term is possible since:

$$-Q_{ik}\alpha_{ik}=Q_{ki}\beta_{ki} \tag{20}$$

and

$$-Q_{ik}\beta_{ik}=Q_{ki}\alpha_{ki} \tag{21}$$

Using equation (19), if the terms containing the dependent variable $N_{1,i}$ are grouped on the left hand side and the direct loads of this component and the terms for the formation of N_1 due to other components are placed on the right hand side, one obtains:(8)

$$a_{ii}N_{1,i}+\sum_k a_{ik}N_{1,k}=W_{1,i}+V_iK_{21}N_{2,i}+\dots+V_iK_{31}N_{3,i}+\dots+V_iK_{51}N_{5,i} \tag{22}$$

where

$$a_{ii}=\sum_k(Q_{ik}\alpha_{ik}+E'_{ik})+V_iK_{11,i} \tag{22A}$$

$$a_{ik}=Q_{ik}\beta_{ik}-E'_{ik} \tag{22B}$$

For sections where flow enters a section from the boundary with a concentration c_b

$$a_{ii}=\sum_k(Q_{ik}\alpha_{ik}+E'_{ik})+V_iK_{11,i}+Q_{ii}\beta_{ii}+E'_{ii} \tag{23}$$

and the forcing function at the boundary is added to the direct loads at that section by:

$$W_{1,i}=W_{1,i}+(E'_{ii}-Q_{ii}\alpha_{ii})c_b \tag{24}$$

For sections forming a boundary, where flow leaves this section to an area with a concentration c_b:

$$a_{ii}=\sum_k(Q_{ik}\alpha_{ik}+E'_{ik})+V_iK_{11,i}+Q_{ii}\alpha_{ii}+E'_{ii} \tag{25}$$

and

$$W_{1,i}=W_{1,i}+(E'_{ii}-Q_{ii}\beta_{ii})c_b \tag{26}$$

The set of equations for component N_1 for n number of spacial sections in the system described in figure 1 would be:

$$a_{11}N_{1,1}+a_{12}N_{1,2}+a_{13}N_{1,3}+a_{14}N_{1,4}+\dots+a_{1n}N_{1,n}=W_{1,1}+V_1K_{21,1}N_{2,1}+V_1K_{31,1}N_{3,1}+\dots+V_1K_{51}N_{5,1} \tag{27}$$

$$a_{21}N_{1,1}+a_{22}N_{1,2}+a_{23}N_{1,3}+a_{24}N_{1,4}+\dots+a_{2n}N_{1,n}=W_{1,2}+V_2K_{21,2}N_{2,2}+V_2K_{31,2}N_{3,2}+\dots+V_2K_{51,2}N_{5,2} \tag{28}$$

$$a_{31}N_{1,1}+a_{32}N_{1,2}+a_{33}N_{1,3}+\dots+a_{3n}N_{1,n}=W_{1,3}+V_3K_{21,3}N_{2,3}+V_3K_{31,3}N_{3,3}+\dots+V_3K_{51,3}N_{5,3} \tag{29}$$

$$a_{n1}N_{1,1}+a_{n2}N_{1,2}+a_{n3}+\dots+a_{nn}N_{1,n}=W_{1,n}+V_nK_{21,n}N_{2,n}+V_nK_{31,n}N_{3,n}+\dots+V_nK_{51,n}N_{5,n} \tag{30}$$

In matrix notation equations (27) thru (30) can be written as:

$$[A_1](N_1)=(W_1)+[VK_{21}](N_2)+[VK_{31}](N_3)+[VK_{41}](N_4)+[VK_{51}](N_5) \tag{31}$$

where:

$[A_1]$ is a square matrix of n order, containing the a's as defined on equations (22A) and (22B), note that the main diagonal has the reaction rate constant K_{11}
$(N_1),(N_2),\dots(N_5)$ are nx1 vectors of the reactant over all sections
(W_1) is an nx1 vector of the waste loads for reactant N_1 for all sections
$[VK_{21}],[VK_{31}],[VK_{41}]$ and $[VK_{51}]$ each of these is an nxn diagonal matrix of the section volume and the first order reaction coefficient at that segment.

A similar analysis as above for the second reactant N_2 on figure 1 yields:

$$[A_2](N_2)=(W_2)+[VK_{12}](N_1)+[VK_{32}](N_3)+[VK_{42}](N_4)+[VK_{52}](N_5) \tag{32}$$

where:

$[A_2]$ is an nxn matrix similar to $[A_1]$, but the main diagonal contains the reaction rate constant K_{22}
(W_2) is an nx1 vector of direct waste loads for component N_2 over the n sections

For the other reactants N_3, N_4, N_5 similar equations are generated:

$$[A_3](N_3)=(W_3)+[VK_{13}](N_1)+[VK_{23}](N_2)+[VK_{43}](N_4)+[VK_{53}](N_5) \tag{33}$$

$$[A_4](N_4)=(W_4)+[VK_{14}](N_1)+[VK_{24}](N_2)+[VK_{34}](N_3)+[VK_{54}](N_5) \tag{34}$$

$$[A_5](N_5)=(W_5)+[VK_{15}](N_1)+[VK_{25}](N_2)+[VK_{35}](N_3)+[VK_{45}](N_4) \tag{35}$$

The above matrix equations (31) thru (35) can be written as a matrix of Matrices:(5,8)

$$\begin{bmatrix} [A_1\ \ ] & -[VK_{21}] & -[VK_{31}] & -[VK_{41}] & -[VK_{51}] \\ -[VK_{12}] & [A_2\ \ ] & -[VK_{32}] & -[VK_{42}] & -[VK_{52}] \\ -[VK_{13}] & -[VK_{23}] & [A_3\ \ ] & -[VK_{43}] & -[VK_{35}] \\ -[VK_{14}] & -[VK_{24}] & -[VK_{34}] & [A_4\ \ ] & -[VK_{54}] \\ -[VK_{15}] & -[VK_{25}] & -[VK_{35}] & -[VK_{45}] & [A_5\ \ ] \end{bmatrix} \begin{pmatrix} (N_1) \\ (N_2) \\ (N_3) \\ (N_4) \\ (N_5) \end{pmatrix} = \begin{pmatrix} (W_1) \\ (W_2) \\ (W_3) \\ (W_4) \\ (W_5) \end{pmatrix}$$

or

$$[\bar{A}]\ (\bar{N}) = (\bar{W}) \qquad \text{.........................} \ (37)$$

where $[\bar{A}]$ is the 5n x 5n matrix above and $(\bar{N})$ and $(\bar{W})$ are 5n x 1 vectors. The solution of the five reactants over all the spacial sections are given by

$$(\bar{N}) = [\bar{A}]^{-1}\ (\bar{W}) \qquad \text{.........................} \ (38)$$

Application of the theory by the computer program

The program described follows a modular approach in which the user specifies to the main line program the options desired, and subroutines are called accordingly to perform specific tasks.

The steps to be accomplished can be summarized as:

a) Input the physical characteristics of the system; namely, the geometry, temperature, hydrologic characteristics, reaction schemes and corresponding reaction rates.
b) Calculate E' and α's for all the sections as described on equations (9C) and (10). In order to handle the constraint stated on equation (12), the program tests the expression:

$$\alpha_{ij} < 1 - E'_{ij}/Q_{ij} \qquad \text{.........................} \ (39)$$

and if such is the case α_{ij} is recalculated as:

$$\alpha_{ij} = 1 - E'_{ij}/2Q_{ij} \qquad \text{.........................} \ (40)$$

which places α_{ij} well within the tolerable range.

c) Set up the system matrix $[A_i]$ by computing its elements as given on equations (22A) and (22B). It should be noted that the difference between the $[A_i]$ matrices in equations (31) thru (35) is the addition of a separate main diagonal term $K_iK_{jj,i}$. In order to conserve space, this matrix is set up without this term and during the creation of the matrix of matrices $[\bar{A}]$, the appropriate $V_iK_{jj,i}$ term is added.
d) Set up the matrix of matrices $[\bar{A}]$, this is done by combining an offline disk file containing all the V_iK_i terms for the system and the $[A_i]$ matrix.
e) Input of direct discharges into the system and boundary concentrations, and from these compute the system source vector (W) as described on equations (24) and (26).
f) Solve for the reactants concentrations at all segments by inverting the matrix $[\bar{A}]$ and multiplying it by the waste vector $(\bar{W})$.

Optionally, the program can also perform system sensitivity analysis by varying the waste vector (W) and re-multiplying by $[\bar{A}]^{-1}$ and/or changing the reaction rate constants for any reactants and repeating step (f). A second option is the computation of dissolved oxygen deficit and the corresponding dissolved oxygen concentration by selecting the reaction schemes producing the deficit and the associated stochiometric coefficient.

The computer program has been written for the IBM 370 with a Fortran (IV) G or H level compiler. The program occupies 140K of core to execute and takes 35 CPU seconds to solve a 10 segment, 8 component system. As presently written, the program can accommodate a multi-dimensional system of up to sixty sections and each section can have a maximum of six interfaces. The maximum number of reactants is such that when multiplied by the number of sections cannot exceed 120. This present limitation can be easily expanded.

Application to nitrification

Figure 4 is a schematic representation of the nitrogen cycle:

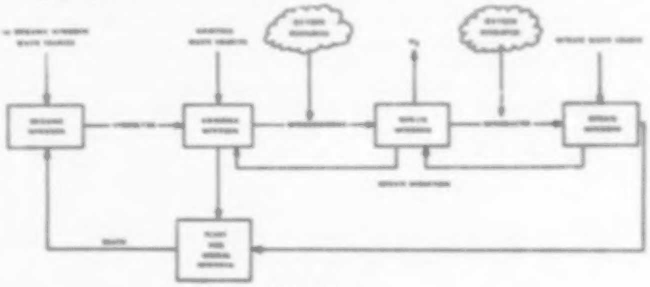

FIGURE 4
MAJOR FEATURES OF THE NITROGEN CYCLE

Since waste loads are usually in the form of organic nitrogen or ammonia, these species will consume oxygen by the bacterial reactions:(7)

$$NH_4^+ + 3/2\ O_2 \xrightarrow[\text{Bacteria}]{\text{Nitrosomas}} NO_2^- + 2H^+ + H_2O \qquad \text{.........} \ (41)$$

followed by

$$NO_2^- + 1/2\ O_2 \xrightarrow[\text{Bacteria}]{\text{Nitrobacter}} NO_3^- \qquad \text{..................} \ (42)$$

From the stochiometry of the reaction on equation (41), it takes 3.43 grams of oxygen for the oxydation of one gram of ammonia as nitrogen to nitrite. The second reaction takes 1.14 grams of oxygen for the oxydation of one gram of nitrite as nitrogen to nitrate. The entire oxydation process therefore takes 4.57 grams of oxygen per gram of ammonia nitrogen.

Letting:

N_1 = organic nitrogen
N_2 = ammonia nitrogen
N_3 = nitrite nitrogen
N_4 = nitrate nitrogen
N_5 = plant and animal nitrogen

The system to be solved would be:

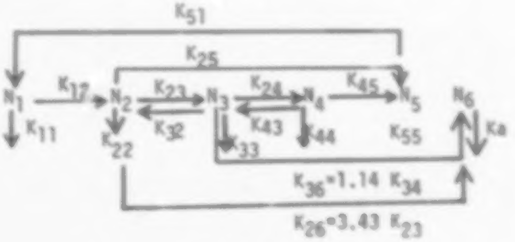

FIGURE 5
NITROGEN CYCLE WITH DEFICIT COMPONENT

If we assume these reactions to follow first order kinetics, the system can readily be solved using program FEDBAK03. The computation of dissolved oxygen deficit can be accomplished two ways. A deficit "species" can be defined (noted N_6 above), the decay of which is the reaeration rate, Ka. The reaction schemes producing deficit are then defined, and the corresponding reaction rate would be the product of the stochiometric coefficient by the reaction rate of the reaction using up oxygen. A second method to compute deficit concentrations as done for component N_1 in equations (22) thru (31), one obtains

$$[B](D)_i=3.43[VK_{23}](N_2)+1.14[VK_{34}](N_3) \ \ldots\ldots \ (43)$$

where [B] is a matrix similar to the $[A_i]$ matrices of equations (31) thru (35), except that the main diagonal term has the reaeration rate Ka instead of K_{ii}. (N_2) and (N_3) are nx1 vectors of the steady-state concentration of these reactants. $(D)_i$ is an nx1 vector of the deficit concentrations over all segments due to the oxydation of ammonia and nitrite. The solution to the deficit concentration over all space is given by:

$$(D)_i=3.43[VK_{23}](N_2)[B]^{-1}+1.14[VK_{34}](N_3)[B]^{-1}. (44)$$

This method is used to compute deficit in program FEDBAK, by using the optional subroutine.

The application to nitrification and dissolved oxygen deficit assumed first order kinetics for the bacterial reactions. This should be confirmed by laboratory studies, or the nature of the system should be carefully considered. This computer model has been found to be very useful as a predictive tool and in providing insights to the behavior of nitrogen species in the aquatic environment. On new applications this will ultimately depend on the applicatively of the underlying assumptions to the system of interest.

ACKNOWLEDGEMENTS

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MODELING THE HYDRODYNAMIC EFFECTS OF LARGE MAN-MADE MODIFICATION TO LAKES

John F. Paul
Department of Earth Sciences
Case Western Reserve University
Cleveland, Ohio 44106
currently at
Large Lakes Research Station
Environmental Research Laboratory-Duluth
Grosse Ile, Michigan 48138

Summary

A three dimensional hydrodynamic model is described which can be used as a predictive tool for assessing the possible effects of large man-made modifications to lakes. The example of the proposed jetport island in Lake Erie is used as a sample application of the model.

Introduction

The real value of numerical models is in their predictive capability. By this is meant their ability to be used for physical situations that are distinctly different from those for which they have been developed. The major use of models has so far been in the verification sense, that is, they have been developed to agree with existing sets of data. The purpose of this paper is to present an example of the predictive use of one particular hydrodynamic numerical model.[1,2,3]

A new jetport has been proposed to be built in the vicinity of Cleveland, Ohio. One possible site being considered is a to-be-built dyked area in Lake Erie near Cleveland. As part of the feasibility studies for the proposed lake jetport, a numerical model describing the hydrodynamics of the Lake Erie area near Cleveland was developed to help determine the possible effects of such a jetport on the summer temperature structure in the lake.

A numerical model for a situation such as the proposed jetport has several advantages. First, once the model is developed, simulations are relatively inexpensive to produce, compared to building and running a physical model or conducting field surveys. For example, the numerical model to be discussed requires approximately twenty minutes of CPU time for one day of real-time simulation. Second, it is extremely easy to simulate different physical conditions on the lake, e.g., different wind directions and speeds, and different thermal structure. Third, it is a simple task to alter the model geometry to simulate the effect of different jetport configurations. In this way the model could be considered as a design tool.

Another advantage of a numerical model is that it may be the only alternative for assessing a proposed modification to a lake. For this jetport example, field data can only be used to tell what is happening in the lake at the present time, not what happens after a jetport is built in the lake. One conception of the jetport is a two mile by three mile island located five miles off Cleveland. No previous experience with modifications of this scale to large lakes is available. A physical model of this situation would be extremely expensive, and even if it were built, its results may be questionable due to the extreme distortion required in the model and the inability to properly represent some of the physical mechanisms occurring in the lake.

Description of the Numerical Model

The equations for the numerical model are derived from the time-dependent, three-dimensional equations of motion for a viscous, heat-conducting fluid. The basic assumptions used in the model are: (a) The Boussinesq approximation is valid. This assumes that density variations are small and can be neglected in the equations of motion except in the gravity term. The coupling between the energy and momentum equations is retained. (b) Eddy coefficients are used to account for turbulent diffusion effects in both the momentum and energy equations. The horizontal eddy coefficients are assumed constant but the vertical eddy coefficients vary depending on the vertical temperature gradient and other parameters. (c) The rigid-lid approximation is valid, i.e., the vertical velocity at the undisturbed water surface is zero. This approximation is used to eliminate surface gravity waves and the small time scales associated with them, greatly increasing the maximum time step possible in the numerical computations. In this approximation, only the high frequency surface variations associated with gravity waves are neglected. (d) The pressure is assumed to vary hydrostatically.

The model equations, as described in detail by Paul and Lick[3], are:

1. the three-dimensional, incompressible continuity equation,
2. two time-dependent, three-dimensional horizontal momentum equations,
3. the time-dependent, three-dimensional temperature equation,
4. the equation of state,
5. the Poisson equation for the pressure.

The boundary conditions used with the above equations are as follows. The bottom and shore are taken as no-slip, impermeable, insulated surfaces. A heat transfer condition proportional to a temper-

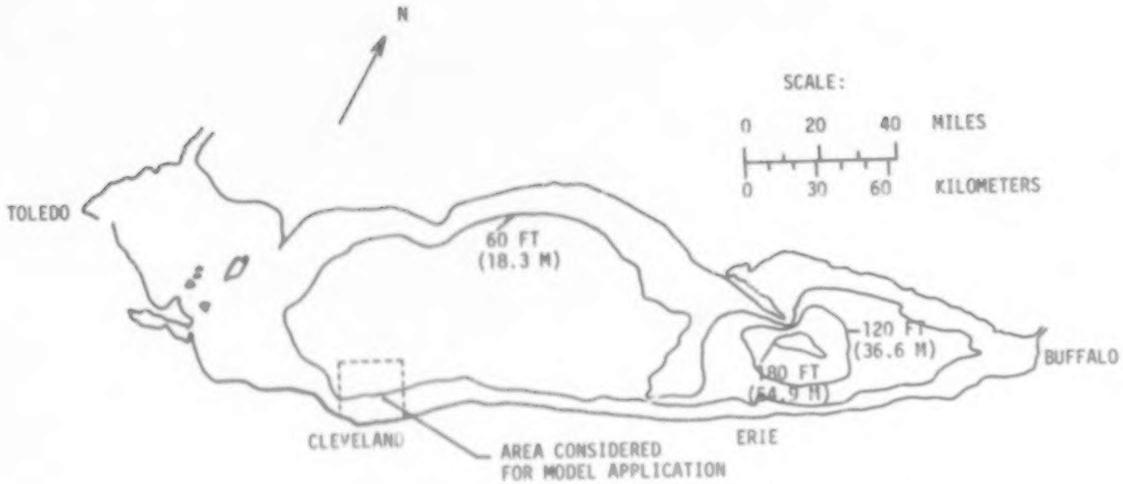

FIGURE 1. AREA OF LAKE ERIE CONSIDERED FOR APPLICATION OF THE MODEL

ature difference[3] and a wind-dependent stress are imposed at the water surface. The pressure boundary conditions are derived from the appropriate horizontal momentum equation. Along the open water boundaries either velocity and temperature values are specified or normal derivatives of the velocity and temperature are set to zero.

The equations and boundary conditions are put into appropriate finite differences form in both space and time. A strictly conservative numerical scheme is used in the model. In addition, a stretching of the vertical coordinate proportional to the local depth is used. With this transformation, the same number of vertical grid points are present in the shallow as in the deeper parts of the lake. This ensures that in the shallow areas there is no loss of accuracy in the computations due to lack of vertical resolution. Refer to the report by Paul and Lick[3] for details.

Application of the Numerical Model to the Jetport

The section of Lake Erie considered is a sixteen mile by sixteen mile area near Cleveland (Figure 1). The jetport configuration used in this example is a two mile by three mile island five miles from Cleveland in approximately fifty feet (15.2 m) of water. The numerical model has been run with and without the jetport island. Sample results are presented for 14.8 hours after the start of a 12 mph (5.4 m/sec) wind from the south. The lake is initially stratified with a thermocline depth of 30 ft (9.15 m), epilimnion temperature of 75°F (24°C), and hypolimnion temperature of 55°F (13°C). Figures 2 through 5 show results without the jetport island and Figures 6 through 9 show results with the jetport island.

Comparing the horizontal isotherm plots (Figures 2, 3, 6, 7) for the two cases, it is apparent that the jetport island influences the temperature of the lake over a large distance (about 6 to 8 miles) from the island. The velocity plots (Figures 4, 5, 8, 9) also indicate a large region of influence. This effect is due to the upwelling of cold water on the eastern edge of the island and downwelling of warm water on the western edge. These upwellings and downwellings result in changes to the stratification structure in that area of the lake. Since this is a variable-density model, changes in the temperature structure do cause changes in the velocity pattern. Using a constant-density, free surface model, Sheng found that the jetport island only exerted [illegible] influence over a distance of one to two miles into the lake.

The results presented are for only one particular wind direction. As the wind shifts, the upwelling and downwelling regions change their positions around the island. Thus, it can be seen that the effect of the proposed jetport island during the summer season would be to erode the thermocline in that area of the lake. The mixing of epilimnion and hypolimnion waters may be considered in one way to be beneficial since it will keep the area of the lake affected from going anoxic in the late summer, but in another way it may not be considered beneficial because of the increased nutrient input to the epilimnion. Also, this forcing of warm water to the bottom may be detrimental to aquatic species dependent upon colder waters for their existence or reproductive activities.

The model also could be used to predict the effect of different jetport configurations, for example, a jetport peninsula instead of a jetport island. The results presented are qualitative and indicate how a numerical model might be used to predict the effects of large man-made modifications to lakes.

Acknowledgement

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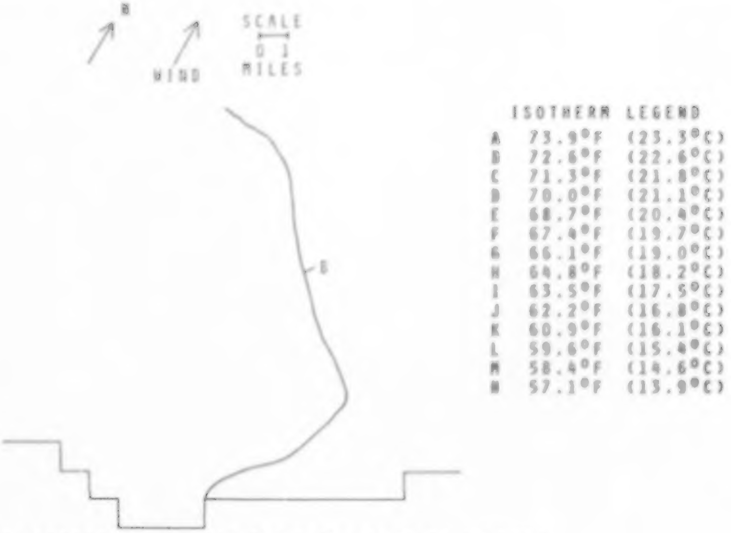

FIGURE 2. SURFACE ISOTHERMS FOR MODEL WITHOUT JETPORT

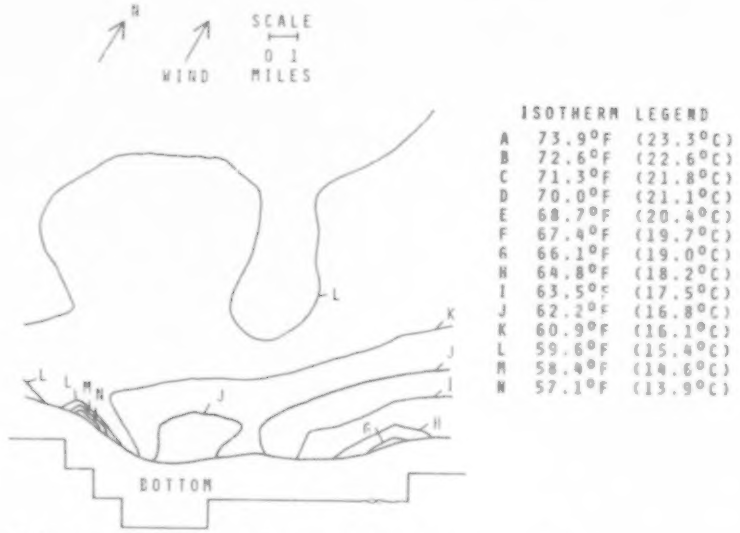

FIGURE 3. ISOTHERMS AT 40 FT FOR MODEL WITHOUT JETPORT

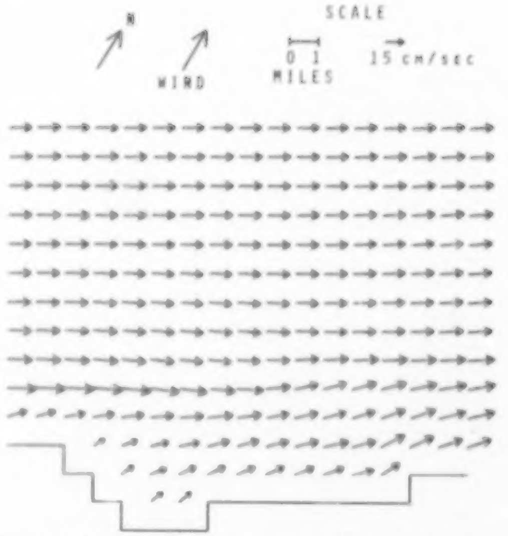

FIGURE 4. SURFACE VELOCITIES FOR MODEL WITHOUT JETPORT

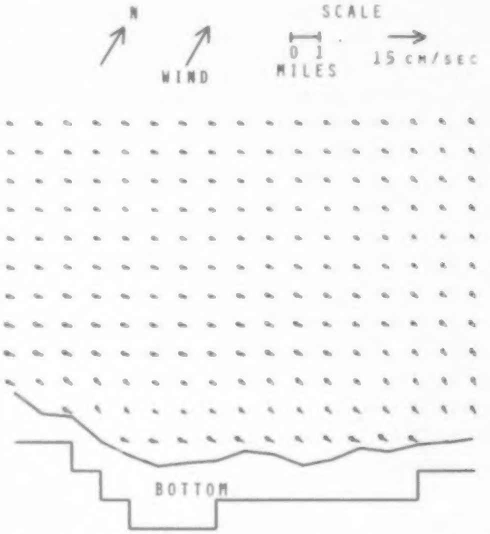

FIGURE 5. VELOCITIES AT 40 FT FOR MODEL WITHOUT JETPORT

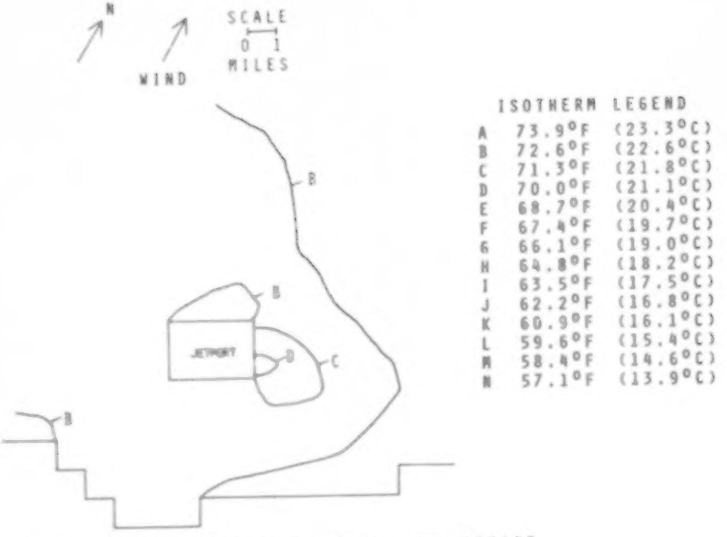

FIGURE 6. SURFACE ISOTHERMS FOR MODEL WITH JETPORT

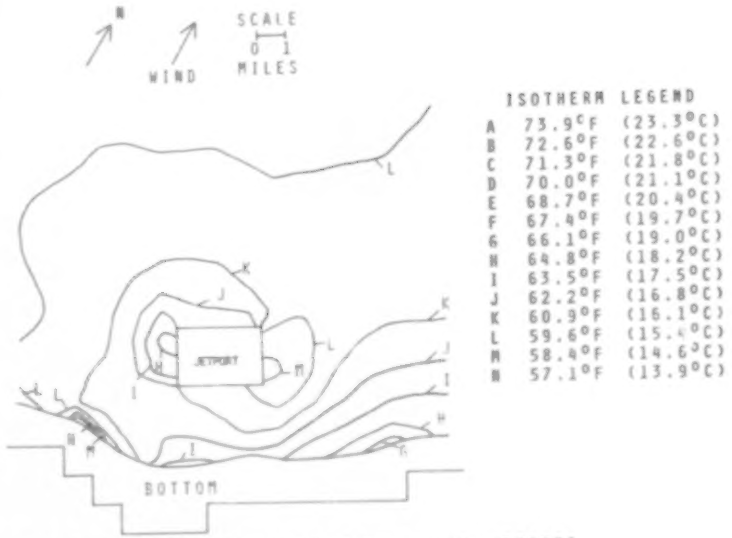

FIGURE 7. ISOTHERMS AT 40 FT FOR MODEL WITH JETPORT

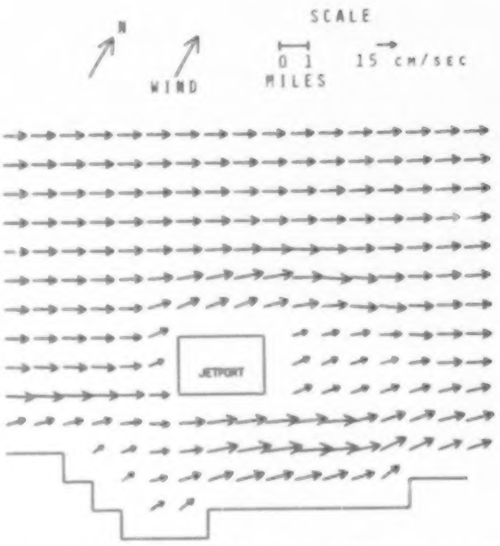

FIGURE 8. SURFACE VELOCITIES FOR MODEL WITH JETPORT

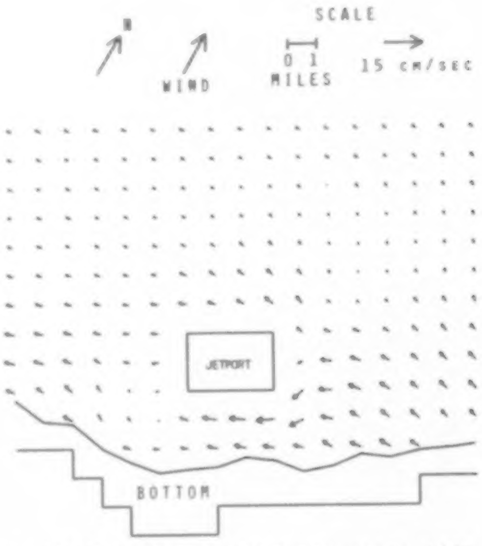

FIGURE 9. VELOCITIES AT 40 FT FOR MODEL WITH JETPORT

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AN EMPIRICAL MODEL FOR NUTRIENT ACCUMULATION RATES IN LAKE ONTARIO

Patricia A.A. Clark
U.S. Environmental Protection Agency
Rochester, New York

Jane P. Sandwick
U.S. Environmental Protection Agnecy
Rochester, New York

Donald J. Casey
U.S. Environmental Protection Agency
Rochester, New York

Anthony Solpietro
U.S. Environmental Protection Agency
Rochester, New York

Abstract

Based on the chemical concentration data collected during the International Field Year for the Great Lakes (IFYGL)--May 1972 through June 1973, monthly average rates of chemical accumulation have been determined for total phosphate (TP), nitrite-nitrate (NO_2-NO_3), ammonia (NH_3), total Kjeldahl nitrogen (TKN), total organic carbon (TOC), and (SO_4). The accumulation rates are the consequence of such processes as biochemical transformation processes, sediment exchanges, etc. The model relates the accumulation rate of a particular substance with the rate of exchange of the total mass of that substance in the lake and with the total net loading rate to the lake (tributaries, direct industrial, direct municipal and on-lake precipitation).

The total masses of each chemical substance for each of the 11 cruises (Figures 1-6) have been calculated using the numerical integration computer program SPLOTCH (Boyce 1973) with the input of concentration measurements which were collected from about 75 stations on the lake at depths of 1,5,10,20,25,30,40,50,100,150 meters and at the lake bottom.[3] This study is described by Casey, Clark and Sandwick (1976) together with the U.S. tributary loading rates and the direct on lake precipitation loading rates.[4] Canadian tributary loading rates for the same period were presented by Casey and Salbach (1975).[5] The mass balance equation relating these quantities and the accumulation rate will now be derived. All quantities in the equation can be evaluated directly on the basis of the measured lake concentrations and loading rates so that the equation can be solved for the accumulation rate in each case. In addition, analysis of the equation will provide a means for the assessment of certain assumptions which are commonly made in large lake limnology.

Accumulation Rate Equation

It is convenient to begin with the hydrodynamic equation for the conservation of mass in the integral form (see, for example, Batchelor 1967),

$$\iiint_V dV \frac{\partial \rho_i}{\partial t} = \oiint_S \rho_i \underline{v} \cdot \underline{n}\, dS + \iiint_V \Sigma_i dV \qquad (1)$$

where ρ_i is the concentration of chemical species i, $\underline{v}$ is the flow velocity and Σ_i is the rate of accumulation (or loss) per unit volume of the same species. V is the volume of the fluid (in this case the volume of Lake Ontario). S is the total surface bounding the volume of the lake.

The term on the left-hand side of eq. (1) can be written as

$$\iiint_V dV \frac{\partial \rho_i}{\partial t} = \frac{d}{dt}\iiint_V dV \rho_i - \iiint_V \rho_i\, d\left(\frac{\partial V}{\partial t}\right) \qquad (2)$$

$$= \frac{dm_i}{dt} + C_i$$

where m_i is the total mass of chemical species i in the lake at time t. C_i designates the second term on the right of eq. (2). This term can be neglected whenever $(\Delta\rho/\rho) >> (\Delta V/V)$. The U.S. Army Corps of Engineers measured a change of about 1 meter in the level of Lake Ontario (Monthly Bulletin of the Lake Levels, 1972 and 1973).[11] This corresponds to a volume increment of about 20 km^3 so that $\Delta V/V \sim .012$. If this is compared with $(\Delta\rho/\rho) \sim .20$ for total phosphate (see Table 1), which has about the smallest concentration variation of any of the chemical substances studied, it is apparent that $(\Delta\rho/\rho) >> (\Delta V/V)$ will hold for all substances.

The second term in eq. (1) is the net loading rate

$$\oiint_S \rho \underline{v} \cdot \underline{n}\, dS = L_i^T + L_i^R + L_i^S \qquad (3)$$

where L_i^T is the net loading rate (inflow minus outflow) due to tributary stream flow, L_i^R is the loading rate due to rainfall directly on the lake surface and L_i^S is the net loading due to sediment (sediment release - sediment adsorption). L_i^T and L_i^R are shown in Tables 1, 3, 4, 6, 7, 9. Calculations of L_i^R are based on precipitation chemistry measurements reported by Shiomi and Kuntz (1973) and by Casey et al., (1975) and monthly total of lake precipitation measured by Bolsenga and Hagman (1975).[10,4,8] L_i^S must be either estimated or calculated.

The third term in eq. (1) is the total net rate of production of species i

$$\iiint \Sigma_i dV = T_i \qquad (4)$$

where T_i is a function of time.

Substituting eqs. (2), (3), and (4) into eq. (1) results in the following equation.

$$\frac{dm_i}{dt} = L_i^T + L_i^R + L_i^S + T_i \qquad (5)$$

All quantities in eq. (5) can be determined from measurements except the sum, $L_i + T_i = S_i$ so this sum can be obtained from equation (5). Eq. (5) may be rewritten as

$$\frac{dm}{dt} = L_i + S_i \qquad (6)$$

where $L_i = L_i^T + L_i^R$

Equation (6) is similar to that obtained by Vollenweider (1969),

$$\frac{dm_w}{dt} = J - \frac{Q}{V} m_w - \sigma m_w \qquad (7)$$

where m_w is the total amount of substance w in the lake at time t, J is the rate of tributary loading of substance w to the lake, Q is the mean discharge out of the lake, V is the mean volume of the lake and σ is the sedimentation rate coefficient.[12]

In comparing eqs. (6) and (7) L_i is the net loading rate (inflow-outflow) obtained directly from measurement. The comparable terms in eq. (7), $J-Qm_w/V$, involve an assumption about the outflow. The actual outflow and the Qm_w/V assumed form are compared. The inclusion of a surface contribution in the source term in these equations seems prudent in view of the discussion by Dillon and Kirchner (1975), Kirchner and Dillon (1975), Dillon (1975) and Chapra (1975) with regard to phosphate.[2,3,5,6]

dm_w/dt is obtained from a numerical differentiation of m_i (t) calculated by means of the SPLOTCH program. It is assumed that the chemical masses so obtained are characteristic of the average chemical masses in the lake for the month during which the cruise occurred. The assumption seems justified on the basis of the relatively smooth progression of mass determinations from cruise to cruise. For those months for which no cruises took place, linearly interpolated values have been obtained. The monthly variations in chemical mass contents of the lake are plotted in Figures 1-6 and will be discussed in the accumulation rates section. Numerical differentiation of m_i with respect to t is performed by passing a parabola through 3 successive monthly mass values, m_1, m_2, m_3. The derivative at the mid point is given by

$$\frac{dm}{dt} = \frac{m_3 - m_1}{2h} + O(h^2) \tag{8}$$

where $h = t_n - t_{n-1}$ (see, for example, Wylie, 1951). In this case h = month, however, dm/dt is expressed in units of metric tons/day. The monthly values of dm/dt for each substance are provided in Tables 2, 5, 8. These tables also include the total monthly loading rate L and the calculated value of the monthly source term S for each substance.

Nutrient Accumulation Rates

For each substance studied, the variation of the mass content is shown and described. A numerical time differentiation of the monthly mass content has been performed and is tabulated. This quantity together with the monthly loading rates to the lake have been substituted into eq. (6) to yield the source term. The nature of the source term variation is discussed in order to extract information regarding the nature of the physical processes.

Using the IFYGL data we have examined the Vollenweider model which assumed a source term of the form, $-\sigma m_w$ (eq. (7)). For each of the 6 substances of this study, the model proved inadequate since the structures of the functions S and m (or m_w) for each substance are very different. The assumed form of the outflow term in eq. (7), Qm_w/V, when compared with the measured St. Lawrence loading proves a useful model for nitrite-nitrate, total Kjeldahl nitrogen, sulfate and organic carbon while in the cases of total phosphate and ammonia, the model predictions deviate considerably from the measured value.

Total Phosphate

The total phosphate content of the lake shows an average pf 9.5% from the mean with a maximum deviation of 19%. The maximum deviations occurred in spring 1972 and 1973 and early winter 1972, reflecting seasonal perturbations from the mean (see Figure 1). Thus dm/dt will be small. Table 1 lists the various contributions and the net total loading rate of total phosphate by month. The total net loading rate to the lake varied by a factor of 10 reaching a maximum in the December 1972 through March 1973 period and a minimum in the August through October 1972 period. Having obtained the mean monthly numerical derivative, dm/dt, and the total net loading rate L, eq. (6) yields the source term. All of these quantities are listed in Table 2.

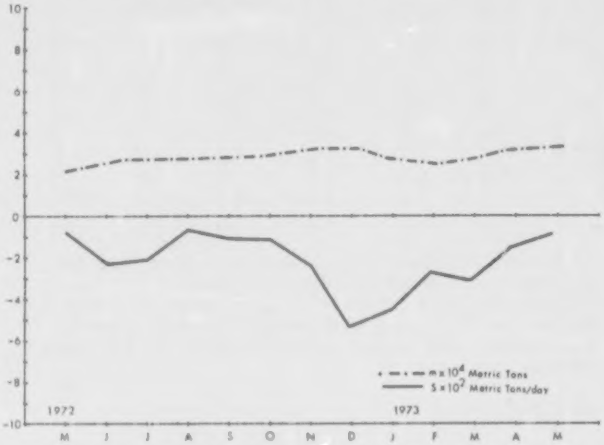

FIGURE 1 THE MASS CONTENT (m) AND THE PRODUCTION RATE (S) OF TOTAL PHOSPHATE DURING THE FIELD YEAR.

Table I - Total phosphate loading rates to Lake Ontario
(metric tons/day)

Month	Niagara River	U.S. Tributaries	Canadian Tributaries	St. Lawrence River
Apr 1972	19.2	18.4	5.1	20.7
May	12.5	12.5	3.9	19.8
Jun	24.0	11.1	3.6	21.7
Jul	20.4	12.7	5.8	27.2
Aug	22.1	4.6	1.9	33.6
Sep	17.2	2.9	1.3	21.6
Oct	15.4	4.8	2.0	16.9
Nov	19.3	9.0	2.2	15.8
Dec	31.5	14.9	4.8	13.3
Jan 1973	18.6	12.5	3.0	12.9
Feb	23.5	8.9	2.6	20.4
Mar	28.9	18.7	5.7	25.4
Apr	17.8	14.2	3.9	27.0
May	14.5	7.7	2.7	28.0
Mean	20.4	10.9	3.5	21.7

Month	Direct municipal and industrial U.S.	Direct municipal and industrial Canada	Direct Precip.	Net loading rate
Apr 1972	.16	8.3	4.9	35.4
May	.14	7.3	6.0	22.5
Jun	.14	7.1	7.9	32.1
July	.15	7.7	4.8	24.4
Aug	.13	6.7	6.4	8.2
Sep	.15	7.9	5.1	13.0
Oct	.14	7.4	5.3	18.6
Nov	.14	7.3	7.9	30.0
Dec	.18	9.1	8.2	55.4
Jan 1973	.18	9.6	2.8	34.6
Feb	.19	9.9	4.0	28.7
Mar	.17	9.0	7.5	44.6
Apr	.16	8.3	7.7	25.1
May	.15	7.9	5.8	10.8
Mean	.16	8.1	6.1	27.4

Table 2 - Total phosphate and nitrite-nitrate - mass balance equation terms (metric tons/day)

	Total Phosphate			Nitrite-Nitrate		
Month	$dm/dt/10^1$	$-L/10^1$	$S/10^1$	$dm/dt/10^3$	$L/10^3$	$S/10^3$
May 1972	1.48	2.25	- .77	-5.60	.09	-5.69
Jun	.88	3.21	-2.33	.87	.28	.59
Jul	.33	2.44	-2.11	- .28	.03	- .31
Aug	.13	.82	- .69	-3.19	.01	-3.20
Sep	.19	1.30	-1.11	-1.63	.06	-1.69
Oct	.65	1.86	-1.21	-1.11	.06	-1.17
Nov	.55	3.00	-2.45	-1.61	.14	-1.75
Dec	.02	5.54	-5.52	.03	.17	- .14
Jan 1973	-1.25	3.46	-4.71	3.06	.15	2.91
Feb	.07	2.87	-2.80	3.14	.07	3.07
Mar	1.19	4.46	-3.27	- .34	.09	- .43
Apr	.92	2.51	-1.59	-2.50	.11	-2.61
May	.08	1.08	-1.00	-2.31	.10	-2.41
Mean	.39	2.68	-2.27	- .88	.10	-.115

Throughout the field year, there is a loss rate for phosphate, -S, which averages 2.27 metric tons/day. This monthly loss rate varies by a factor of about 7 during the field year with maximum losses occurring in the winter. The August through October period shows a minimum loss rate.

Nitrite-Nitrate

The total nitrite-nitrate content of the lake shows very definite seasonal variation (see Figure 2). Maximum mass content is characteristic of the early summer 1972 and spring 1973 periods with a low occurring in the late summer through fall period. The range of variation is a factor of about 2.3. In Table 3 a compilation of the partial and net total loading rates for NO_2-NO_3 is provided. This net total loading rate varied by a factor of more than 20 during the field year, but is typically more than an order of magnitude smaller than either dm/dt or S. This indicates that a major source of nitrite-nitrate variation is due to the biochemical transformation rather than loading rate variations.

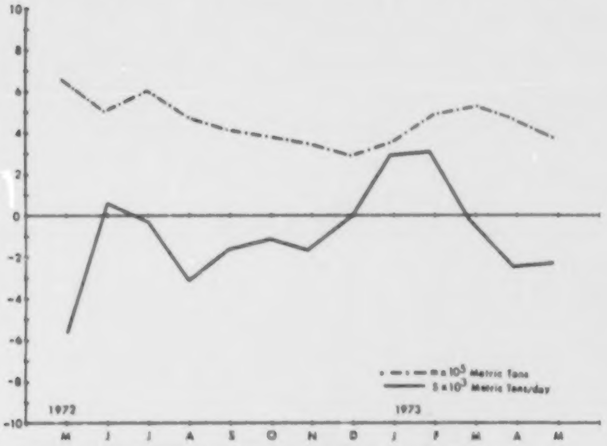

FIGURE 2 THE MASS CONTENT (m) AND THE PRODUCTION RATE (S) OF NITRITE-NITRATE DURING THE FIELD YEAR.

In contract to total phosphate, the source term changed sign during the year so that losses of NO_2-NO_3 occurred in the spring and summer and production was noted during the winter months.

Table 3 - Nitrite-nitrate loading rates to lake Ontario (metric tons/day)

Month	Niagara River	U.S. Tributaries	Canadian Tributaries	St. Lawrence River
Apr 1972	116.2	85.7	17.3	100.0
May	112.7	57.3	11.9	158.6
Jun	182.9	62.6	15.4	62.6
Jul	122.1	63.9	17.6	222.5
Aug	93.9	16.5	3.5	169.7
Sep	24.6	8.3	1.5	29.0
Oct	41.2	13.3	2.2	60.3
Nov	93.6	46.5	9.7	90.9
Dec	130.5	73.1	16.1	108.2
Jan 1973	175.4	64.7	14.2	136.2
Feb	133.8	57.8	14.5	181.7
Mar	153.3	98.1	22.2	258.4
Apr	137.2	77.5	17.1	198.9
May	218.7	36.6	8.5	226.5
Mean	124.0	54.4	12.3	143.1

Month	Direct municipal and industrial U.S.	Direct municipal and industrial Canada	Direct Precip.	Net loading rate
Apr 1972	.47	2.3	49.2	171.2
May	.44	2.2	60.7	86.6
Jun	.42	2.1	79.4	280.2
Jul	.39	1.9	48.5	31.9
Aug	.35	1.7	64.8	11.1
Sep	.35	1.7	51.7	59.2
Oct	.38	1.9	58.0	56.7
Nov	.40	2.0	80.1	141.4
Dec	.54	2.7	58.0	172.7
Jan 1973	.49	2.4	28.7	149.7
Feb	.53	2.6	40.2	67.7
Mar	.54	2.7	75.9	94.2
Apr	.54	2.7	78.1	114.2
May	.48	2.4	58.0	98.2
Mean	.45	2.2	59.4	109.6

Ammonia

The total ammonia content of the lake shows a strong seasonal variation (Figure 3). Highest mass content occurred in the late summer through fall of 1972. After reaching a midwinter minimum, the mass content climbed with onset of spring 1973. Provided in Table 4 are the loading rate contributions of ammonia, which show a variation by a factor of about 3 during the field year.

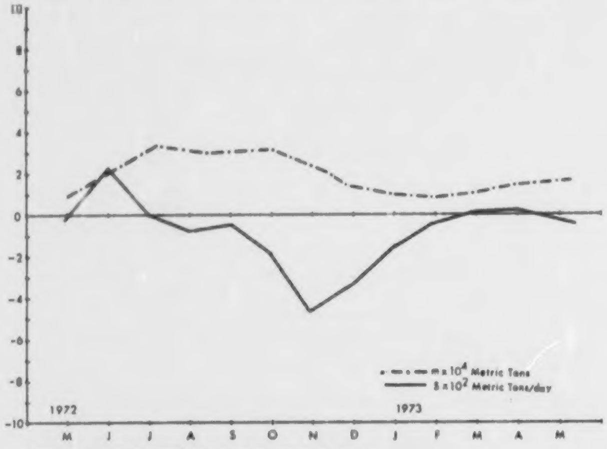

FIGURE 3 THE MASS CONTENT (m) AND THE PRODUCTION RATE (S) OF AMMONIA DURING THE FIELD YEAR.

Tab.[illegible] - Ammonia loading rates to Lake Ontario
(metric tons/day)

Month	Niagara River	U.S. Tributaries	Canadian Tributaries	St. Lawrence River
Apr 1972	27.8	16.2	4.5	3.3
May	16.0	9.9	2.7	4.4
Jun	47.5	13.7	4.7	12.5
Jul	33.3	10.1	3.4	29.2
Aug	27.6	3.9	1.3	32.8
Sep	17.7	2.6	.85	13.0
Oct	17.2	6.1	2.2	11.3
Nov	60.7	17.8	6.5	11.1
Dec	14.4	19.0	6.5	13.0
Jan 1973	30.5	15.4	5.1	19.2
Feb	9.5	13.5	4.7	26.5
Mar	20.8	18.6	5.7	36.4
Apr	15.4	14.6	4.3	27.8
May	12.0	9.8	3.4	16.5
Mean	25.0	12.2	4.0	18.4

Month	Direct municipal and industrial U.S.	Direct municipal and industrial Canada	Direct Precip.	Net loading rate
Apr 1972	3.5	31.4	31.0	111.1
May	2.9	25.9	38.3	91.3
Jun	3.0	25.9	50.0	132.5
Jul	2.6	23.7	30.8	74.5
Aug	2.5	22.6	40.9	66.0
Sep	2.4	20.7	33.7	65.0
Oct	2.5	22.6	36.6	75.9
Nov	3.5	31.8	50.5	159.5
Dec	3.5	31.1	52.2	113.7
Jan 1973	2.8	25.6	18.1	78.3
Feb	3.0	27.1	25.4	58.7
Mar	3.3	30.0	47.9	89.9
Apr	3.4	30.6	49.2	89.7
May	3.0	27.0	36.8	75.3
Mean	3.0	26.9	38.6	91.4

Because of the comparable sizes of the 3 terms in eq. (6) (see Table 5), loadings as well as such processes as biochemical transformation and sediment exchange are important to changes in the ammonia mass content of the lake.

Table 5 - Ammonia and total Kjeldahl nitrogen - mass balance equation terms (metric tons/day)

	Ammonia			Total Kjeldahl Nitrogen		
Month	$dm/dt/10^2$	$L/10^2$	$S/10^2$	$dm/dt/10^3$	$L/10^3$	$S/10^3$
May 1972	.93	.91	.02	.53	.18	.35
Jun	3.62	1.32	2.30	.74	.09	.75
Jul	.81	.75	.07	.00	.13	- .13
Aug	- .10	.66	- .76	- .87	.14	-1.01
Sep	.25	.65	- .40	-1.10	.02	-1.12
Oct	-1.10	.76	-1.86	-1.75	.01	-1.76
Nov	-3.15	1.60	-4.75	-1.31	.17	-1.48
Dec	-2.38	1.14	-3.52	- .10	.23	- .33
Jan 1973	- .84	.78	-1.62	.18	.16	.02
Feb	.13	.57	- .44	- .22	.13	- .35
Mar	1.01	.90	.11	- .76	.19	- .95
Apr	1.17	.90	.27	- .21	.21	- .42
May	.56	.75	- .19	.48	.18	.30
Mean	.07	.90	- .83	- .33	.14	- .47

Total Kjeldahl Nitrogen

Figure 4 shows the seasonal variation of the total Kjeldahl nitrogen content of Lake Ontario during the field year. High values were characteristic of the summer 1972 followed by low levels during the winter and spring 1973. A variation by a factor of 20 occurred in the total net loading rate (see Table 4), L.

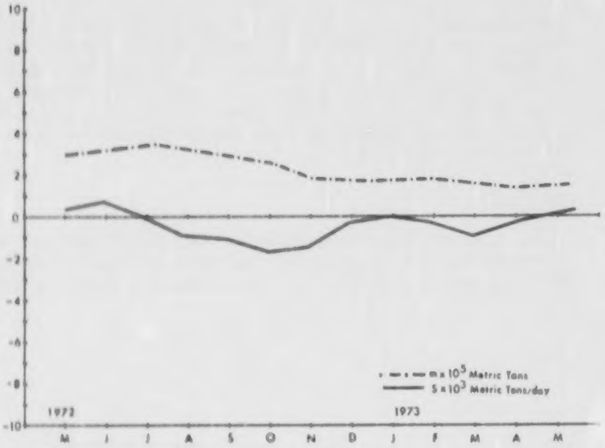

FIGURE 4 THE MASS CONTENT (m) AND THE PRODUCTION RATE (S) OF TOTAL KJELDAHL NITROGEN DURING THE FIELD YEAR.

As is indicated in Table 6 a considerable difference in the relative sizes of dm/dt, L and S was noted during the field year. In spring 1972, winter and spring 1973 the magnitudes of the three terms are comparable while during the summer and fall L is smaller in order of magnitude than dm/dt and S. Thus the biochemical transformations and sediment exchange processes are the

Table 6 - Total Kjeldahl nitrogen loading rates to Lake Ontario
(metric tons/day)

Month	Niagara River	U.S. Tributaries	Canadian Tributaries	St. Lawrence River
Apr 1972	117.3	64.3	36.0	98.4
May	89.8	44.3	36.6	85.7
Jun	91.6	46.8	42.9	204.6
Jul	110.0	42.6	45.0	153.2
Aug	138.0	18.9	18.5	128.4
Sep	124.5	10.3	10.5	211.3
Oct	85.9	18.0	18.1	197.9
Nov	92.9	42.4	36.0	117.5
Dec	109.2	55.8	42.4	106.3
Jan 1973	93.9	51.8	41.9	99.1
Feb	106.5	39.1	33.2	130.1
Mar	107.6	60.8	33.5	132.4
Apr	115.8	49.2	26.5	98.7
May	113.5	31.3	28.2	89.7
Mean	106.9	41.0	32.1	132.4

Month	Direct municipal and industrial U.S.	Direct municipal and industrial Canada	Direct Precip.	Net loading rate
Apr 1972	5.2	41.8	47.4	213.6
May	4.4	35.0	58.5	182.9
Jun	4.5	35.6	76.5	93 3
Jul	3.9	31.5	46.8	126.6
Aug	3.7	29.6	62.5	141.8
Sep	3.6	29.0	51.5	18.1
Oct	3.7	28.1	55.9	11.8
Nov	5.3	30.1	77.2	166.4
Dec	5.2	40.9	79.7	226.9
Jan 1973	4.3	34.5	27.6	154.9
Feb	4.5	36.6	38.8	128.6
Mar	5.1	40.4	73.2	188.2
Apr	5.1	41.2	75.3	214.4
May	4.5	36.0	55.9	179.7
Mean	4.5	35.0	59.1	146.2

dominant sources for changes in the TKN content of the lake during the summer-fall period while loading contributions became more important in the winter and spring. The TKN source term, S, in eq. (6) changes sign during the year with losses indicated in the late summer through winter periods and production in both spring 1972 and 1973.

Sulfate

May, June and July measurements are missing because of difficulties in the chemical analysis of these samples. Sulfate mass content of the lake remained fairly uniform throughout the field year so that dm/dt ≈ 0. This then required a balance between S and L. On the basis of the source term, Table 7 shows sulfate utilization in the summer through fall period and sulfate production in the winter.

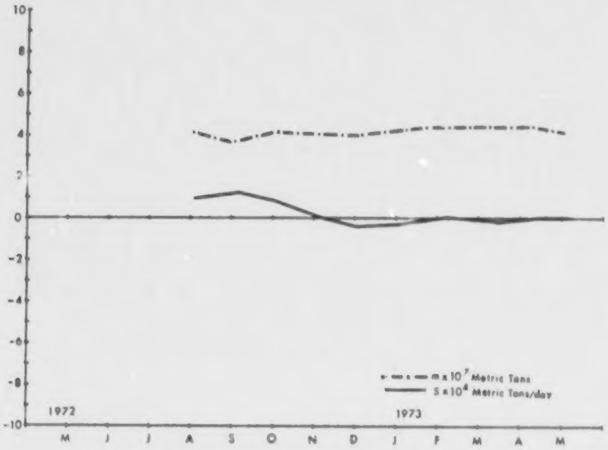

FIGURE 5 THE MASS CONTENT (m) AND PRODUCTION RATE (S) OF SULFATE DURING THE FIELD YEAR.

Table 7 - Sulfate loading rate to Lake Ontario (metric tons/day)

Month	Niagara River	U.S. Tributaries	Canadian Tributaries	St. Lawrence River
Apr 1972	---	---	---	---
May	---	---	---	---
Jun	---	---	---	---
Jul	---	---	---	---
Aug	6609	1327	656	18394
Sep	6843	731	358	20110
Oct	11507	948	419	21043
Nov	16120	2815	1243	21448
Dec	15822	4080	1822	17529
Jan 1973	14163	3605	1604	16340
Feb	14259	2855	1311	17795
Mar	14732	4373	1786	19521
Apr	14961	3260	1262	20680
May	15149	2899	1348	19771
Mean	13016	2869	1181	19283

Month	Direct municipal and industrial U.S.	Direct municipal and industrial Canada	Direct Precip.	Net loading rate
Apr 1972	---	---	---	---
May	---	---	---	---
Jun	---	---	---	---
Jul	---	---	---	---
Aug	27.3	132	506	- 9047
Sep	27.0	130	491	-11530
Oct	27.5	132	533	- 7477
Nov	38.9	187	736	- 308
Dec	38.5	186	760	5180
Jan 1973	31.6	153	263	5480
Feb	32.4	157	370	1189
Mar	37.1	179	698	2105
Apr	37.6	181	717	- 261
May	33.0	159	533	150
Mean	33.1	160	501	-1852

Table 8 - Sulfate and total organic carbon - mass balance equation terms (metric tons/day)

Month	Sulfate dm/dt/10	Sulfate $L/10^5$	Sulfate $S/10^4$	Total Organic Carbon dm/dt/10	Total Organic Carbon $L/10^4$	Total Organic Carbon $S/10^4$
May 1972	----	----	----	1.35	.20	1.15
Jun	----	----	----	4.63	.04	4.59
Jul	----	----	----	2.76	.15	2.61
Aug	----	- .09	.09	.23	.18	.05
Sep	0	- .12	.12	- .31	-.02	- .29
Oct	0	- .07	.07	-1.39	-.11	-1.28
Nov	0	.00	.00	-3.69	.03	-3.72
Dec	0	.05	- .05	-4.66	.23	-4.89
Jan 1973	0	.03	- .03	-2.76	.24	-3.00
Feb	0	.01	- .01	.89	.18	.70
Mar	0	.02	- .02	1.48	.32	1.16
Apr	0	.00	.00	.89	.24	.65
May	0	.00	.00	1.85	.19	1.67
Mean	0	- .01	.01	.10	.14	- .46

Total Organic Carbon

Strong seasonal variations in the total organic carbon content of the lake are illustrated in Figure 6. Peaking in the summer-fall 1972 period, the TOC content fell to a midwinter minimum before beginning a gradual spring rise. A comparison of the terms in eq. (6) as shown in Table 9 indicates that the main balance was between dm/dt and S since L was an order of magnitude smaller. Thus changes in the TOC content of the lake are mainly a consequence of biochemical transformations rather than loading rate differences.

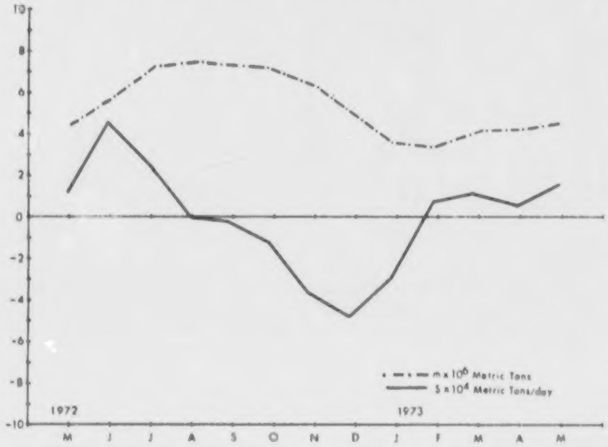

FIGURE 6 THE MASS CONTENT (m) AND THE PRODUCTION RATE (S) OF TOTAL ORGANIC CARBON DURING THE FIELD YEAR.

Table 9 - Total organic carbon loading rates to Lake Ontario (metric tons/day)

Month	Niagara River	U.S. Tributaries	Canadian Tributaries	St. Lawrence River
Apr 1972	1478	714	930	1667
May	2075	525	716	1921
Jun	1323	369	480	2604
Jul	1925	379	531	1894
Aug	2557	325	502	2233
Sep	1874	281	450	3320
Oct	1051	317	487	3562
Nov	298	422	717	1935
Dec	1067	519	672	813
Jan 1973	1884	377	458	651
Feb	1838	255	302	1002
Mar	2102	468	509	647
Apr	2382	364	397	1591
May	2400	280	376	1812
Mean	1732	400	538	1832

Month	Direct municipal and industrial U.S.	Canada	Direct Precip.	Net loading rate
Apr 1972	48.9	54.2	448	2006
May	40.3	44.2	552	2032
Jun	41.7	45.7	722	377
Jul	36.7	40.5	441	1459
Aug	34.5	37.9	590	1813
Sep	33.5	37.2	486	- 158
Oct	34.6	37.9	528	-1107
Nov	49.1	54.2	729	334
Dec	50.1	53.7	753	2302
Jan 1973	39.5	43.6	261	2412
Feb	41.9	46.2	366	1847
Mar	46.7	51.8	691	3222
Apr	46.9	51.6	710	2361
May	41.5	45.5	528	1859
Mean	41.9	46.0	558	1483

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MODELS FOR EXTRAPOLATION OF HEALTH RISK

William M. Upholt
Environmental Protection Agency
Washington, D.C.

Extrapolation models for estimating the risk of adverse effects on human health resulting from low dosages of radiation to which man may be exposed may assume a threshold dosage below which the risk becomes vanishingly low. Aside from theoretical considerations such an assumption is not particularly helpful unless there is a reasonable basis for estimating at what dosage that threshold exists. Moreover, to be most useful in considering the balance between risk and social cost of regulation, the model should provide both a best estimate of risk and an estimate of confidence in that estimate.

Background

Historically, it has been the practice for regulatory agencies to attempt to assure the public that they can promise safety from adverse health effects caused by the toxicants they are regulating. This concept was challenged in the case of ionizing radiation in the first instance and in the case of chemical carcinogens more recently. In both cases it was claimed that there is no reason to assume a threshold and, therefore, there can be no safe dosage. The regulators of radiation realized very early that there was no way to completely eliminate all exposure to ionizing radiation and so they were forced to regulate at exposure levels of acceptable risk rather than no risk. In the case of chemical carcinogens, there is still a strong opinion that no preventable exposure is acceptable and thus complete elimination of all exposure to any controllable carcinogen is the only regulation that is acceptable. Nevertheless, for a number of years some scientists have recognized the difficulties of completely eliminating all exposure to certain carcinogens and so they attempted to define an acceptable risk as one that is mathematically "virtually zero." This "virtual zero" may be 10^{-9}, 10^{-11}, or some other figure depending, presumably, on the size of the population at risk.

A more recent school of regulatory decision-makers insists that the determination of an "acceptable risk" depends in part upon the cost of achieving a lower risk. Thus, according to this school, some form of cost/benefit balancing is necessary to rational decision-making. For purposes of this paper the latter position is taken.

Cost/Benefit Balancing

It is not within the scope of this paper to discuss the many models for decision-making. Neither is the use of the term cost/benefit balancing intended to refer necessarily to costs and benefits in common units and thus arrive at a critical equation for making the regulatory decision. Rather it implies only that both costs and benefits must be considered by the decision-maker before he arrives at his final decision. No specific units are prescribed nor is it necessary to use the same units for both costs and benefits. In fact, it may be undesirable to use dollars or equivalents because of the psychological implication of equating human health to dollars. It is even possible in some cases to describe costs or benefits or both in non-numerical but quantitative terms such as "less than background" or to compare them with other more familiar but similar costs or benefits. Nevertheless, for modeling purposes, at least, it is desirable to strive for understandable numerical terms.

Of course, both costs and benefits may be reversed depending upon the viewpoint of the observer. Even the same observer may reverse the terms from time to time depending upon how he views the decision he is about to make or the audience to which he is addressing his argument. To avoid needless confusion in this paper I have arbitrarily chosen the viewpoint that one purpose of the Environmental Protection Agency is to reduce risk of adverse health effects and thus any reduction in risk that can be attributed to a regulatory action is a benefit. To complete this rationale, the deprivation sustained by society in having to do without the product in question or the increased cost of the product associated with complying with the regulation is the cost to society of achieving the reduced risk.

Threshold Concepts

Accepting the rationale that costs of regulating a product must be justified in terms of reduction in risk does not eliminate the usefulness of the concept of a threshold.

A threshold is normally defined as the lowest dosage at which a given effect is produced. If the effect is one commonly found in the population even in the absence of the substance in question then the threshold becomes the lowest dosage at which the frequency of the effect rises above the background level. Such a point is difficult or impossible to determine experimentally because of the principles of variability and the empirical limits to the size of experimental populations. Thus, it can best be approximated by using a suitable model for extrapolation from points more easily determined experimentally. Though it is always simpler to build a model based upon a smooth continuous curve, it is more important that the model approximate the empirical evidence. Thus, if there is adequate evidence of an unexplained or unanticipated break or other irregularity in the slope of the curve, the model should be modified to accommodate such empirical evidence if it is to be of maximal usefulness in the very practical world of regulation.

There is a concept of long standing in toxicology that effect of a toxicant depends upon dosage. This does not mean that higher dosages necessarily produce more severe or more frequent effects, though this is often true. For instance, if the effect in question is delayed in its development, higher dosages may produce a more serious effect such as death which prevents the development of the effect in question. Actually, it is quite common for a substance to have a reversal in type of effect at extremely low dosages as compared to much higher dosages. Thus it is well known that odors that are strongly attractive at very low dosages may be very repugnant at higher dosages. It is also true that substances such as vitamins that are essential to good health at low dosages may be toxic at high dosages. For such substances it is reasonable to assume that a dose/response curve will go through an inflection point where the slope changes from negative to positive if frequency of adverse effect is shown on the ordinate and dosage on the abscissa. Such a point might well be considered as a threshold even though there is a background of effects from other causes which means that the curve never crosses the x-axis. Since, in such cases, the adverse effect from very low dosages is apt to be different, and possibly independent of the adverse effect at higher dosages, it is probably more reasonable to consider this point an intersection of two curves relating effects of the substance caused by different mechanisms.

Clearly there may also be theoretically sound mechanisms for a positive intersect with the X-axis and also for inflection points showing a sharp change in slope. Thus, the observed effect of a substance may require a two-stage metabolic reaction within the body or a natural defense mechanism may be far more effective at very low dosages than at even slightly higher dosages. For instance, the normal organism may have an excess of cholinesterase that prevents cholinergic symptoms at relatively low dosages of cholinesterase inhibitors, but once the excess is exhausted, the development of cholinergic symptoms occurs over a very narrow range of increased dosages. The observed symptoms may thus have an apparent threshold even though the cholinesterase inhibition curve may have quite a different slope with no distinct threshold.

Models for Extrapolation of Risk

Traditional Threshold Model

Faced with the need for estimating risk at the relatively low dosages to which human populations are exposed, and the frequent necessity to conduct toxicity testing at much higher dosages, a regulatory agency has no alternative but to rely upon extrapolation by means of some model relating dosage to effect, unless it finds it possible to completely stop all exposure to the substance being regulated (or alternatively decides to take no regulatory action). Faced with this problem and the social demands for "safety," regulatory agencies have long found it convenient to assume that there is a threshold or true "no effect" level for any particular adverse health effect and that levels producing no observed effects in experimental animals are a reasonable approximation to that true threshold. Recognizing the realities of experimental variance and limited numbers of experimental subjects, a compensatory "safety" factor was introduced to assure that the standard for regulation was at or below the true threshold. The size of this factor depends upon the same factors that affect experimental variance (size and uniformity of test population and variability between replications in the same and different laboratories). In addition, another factor was added to cover the undetermined physiological differences between man and the experimental organism. The size of this factor might depend upon whether or not there is evidence of human exposure and other aspects of our knowledge of the comparative physiology and toxicology between the species involved.

This model for estimating risk to human populations has been satisfactory in those cases where the cost to society from the resulting regulations has not been exorbitant and the adverse effects have rarely been observed in man. It does not provide a quantitative estimate of risk, nor of benefit of the regulation in terms of reduced risk, and therefore is not very helpful in determining whether or not the societal cost of the regulation is reasonable. Thus, it encourages over-regulation when the adverse effect is easily detected and immediate but it encourages under-regulation when the adverse effect is delayed or otherwise difficult to associate with human exposure.

It is the latter aspect of this type of extrapolation model that has led to a demand that a different model, namely a model which postulates no threshold, be used for regulating substances suspected of causing cancer or other adverse effects that may have an obscured cause. Unfortunately, many individuals have combined this very rational demand for a "no threshold" model with the less rational desire for absolute safety and concluded that the only acceptable standard for such effects is zero exposure or as near to that as can be achieved in the real world.

Interestingly, the other aspect of the traditional "threshold" model (that it encourages over-regulation of substances causing readily apparent adverse effects) also should have led to demand for a more realistic model that would provide a more quantitative estimate of risk, thus reducing societal cost of needless over-regulation.

No Threshold Models

The assumption of no threshold demands more emphasis on the shape of the dose/response curve and its position as related to the axes. It also requires a clearer description of the effect to be assessed and the time at which the effect is to be observed. In the case of a delayed effect such as cancer, it may be a problem to maintain the experimental animals alive long enough for the cancer to be observed. This period often approaches the life expectancy of the unexposed animals. Even at such a termination of observation, the effect seen may not be an obvious cancer but rather a neoplasm that must be carefully examined and classified by an experienced pathologist. If some other effect such as a benign tumor can be described as a precursor to the adverse effect of principal concern (such as cancer) then it is possible to consider this as the effect to be observed. On the other hand, there should be a clear distinction made between various effects in describing the extrapolation model. Thus, if the experimental end point is to be cancer at 24 months of exposure, then a benign tumor that might become malignant at 30 months does not meet the definition. If, on the other hand, benign tumors at 24 months is the end point then that could well include frank cancers (presumably developed from the benign tumors) as well as earlier deaths if benign tumors were present at death. Some statisticians have attempted to develop extrapolation models that take "time-to-cancer" into account since there is experimental evidence that the latent period of cancer is longer at lower levels of exposure. Even in the case of relatively acute effects, the presence of precursors to the adverse end effect must be clearly recognized and considered in developing an extrapolation model. For instance, in the case of cholinesterase inhibition, mentioned above, the adverse health effect of major concern may be serious cholinergic symptoms. Such symptoms, though clearly recognizable, may not be defined easily. It is common to use depression of cholinesterase activity in peripheral blood as a more reproducible end point. However, significant depression in such activity may be detected in the absence of symptoms, and, because cholinesterase can be readily regenerated in the normal body, a low but detectable level of cholinesterase may be of no particular concern.

It is possible to carry this argument to the extreme in which it can be claimed that any foreign substance reaching a living cell will produce some reaction in that cell and thus there is no possible "no-effect" level of exposure that results in such contact with a cell. The conclusion is simply that the end effect of concern must be clearly defined as well as the point in time at which it is to be observed.

Having agreed upon the definition of the effect to be observed and the period of observation, the simplest extrapolation model is a straight line on an arithmetic scale intersecting the origin (in the case of a "no threshold" model) and some observable or experimentally determined point. This model recognizes the principle that frequency of effect usually increases as dosage increases. It ignores experience that shows that the most common curve relating observed effects to dosage is sigmoid in shape. C.I. Bliss[1] developed a widely acclaimed model for use in the experimental range that used probability units (standard deviation using five as the arbitrary unit for 50 percent effect) as the ordinate and the logarithm of the dosage as the abscissa. This model often produces a satisfactory straight line in the usual experimental range of 30 percent to 70 percent effects. Mantel and Bryan[2] used this relationship as the basis for their model but they chose to use a slope of one regardless of the experimental slope (which is frequently greater than one) on the basis that extrapolation is always dangerous so one should be conservative in the sense of minimizing the risk of underestimating the probability of effect at any given dosage. For the same reason, they chose as a determinant point for their model the upper 99 percent confidence limit for the estimate of probability of effect at the highest dosage tested at which no effect was observed.

Numerous other models have been designed in an effort to accommodate certain other observed and theoretical characteristics of the dosage/response relationship. Most of these models agree quite well with observed points (which are usually in the range of 30 percent to 70 percent response, except for those that are either 0 percent or 100 percent) but diverge considerably at very low levels--those levels of greatest concern to the regulatory agencies.

It is perhaps surprising that most modelers have chosen to adopt a series of assumptions, as did Mantel and Bryan, described as conservative and designed to avoid underestimating the risk at any particular dosage. Probably this can be explained on the basis that they have been more concerned with the risk of adverse effects than they have been with cost to society. This is perhaps characteristic of an affluent society that is accustomed to buying what it wants with little concern for cost. It appears less desirable in a regulatory agency charged with protecting society from adverse effects without upsetting the economy. Thus over-conservatism as expressed above can result in major economic problems and even in reducing availability of certain products that society has come to consider essential. This becomes more dramatic when societal cost is expressed in terms of more expensive automobiles, more expensive energy, less plastics, and less ease and rapidity of mobility. Since these are factors that are a part of societal cost which may be required to reduce incidence of cancer and other adverse health effects, and since society does not seem to be willing to pay such costs needlessly, it becomes increasingly important for regulatory agencies to be realistic in their extrapolations rather than "conservative" as that term is used to describe a bias.

Conclusions

It is becoming more important that regulatory agencies consider societal cost of their regulations as well as benefits to society in terms of less risk of adverse health effects. Since the risk can seldom be estimated directly from experimental data based upon relatively high dosages, it is essential that such agencies make judicious use of extrapolation models, always bearing in mind the obvious dangers of extrapolation.

Extrapolation models should provide estimates of two parameters just as is expected of many statistical models. First they should provide a best estimate of the probability of adverse effect at the dosage under consideration. These dosages should include the dosages to which various segments of the population are exposed in the absence of regulation and they should also include dosages that would be expected if various alternative regulatory actions were in fact taken.

It should be borne in mind that such alternatives are typically discrete; that is to say that they are, in the last analysis, dependent upon some form of technology which will reduce pollution to a fixed degree rather than to a continuously variable range. Thus, the dosages that should be considered are a discontinuous set or a step function. They are, therefore, the independent variable, and the probability of adverse effect is the dependent variable. There is little value in selecting arbitrarily a "safe" probability of risk and then designing the technology and regulations to match it. The value or benefits attributable to each alternative regulatory option is thus the reduction of risk that can be expected therefrom.

Secondly, the model should provide an estimate of the degree of uncertainty associated with the estimate of risk. Since, by definition, there is no experimental data in the region of extrapolation, there can be no experimental second moment about the mean and thus no standard deviation in the classical sense. To assume some such figures may well lead to a false confidence in extrapolation. It is most reasonable, then, to be content with a verbal description of uncertainty of the estimated risk. This can be done, possibly by indicating what estimates would have resulted from other assumptions such as the "conservative" assumptions now commonly used. With more experience it may be possible to develop other estimates of uncertainty that are more meaningful to the decision-maker. In any case a "best estimate" of risk or reduction in risk coupled with meaningful disclaimers of accuracy, preferably in terms of describing some of the estimates from alternative assumptions, is preferable to purely subjective guesses either by the decision-maker, or by some expert who very likely has already made up his mind as to the degree of regulation that is justified.

References

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USE OF MATHEMATICAL MODELS IN NONIONIZING RADIATION RESEARCH

Claude M. Weil
Experimental Biology Division
Health Effects Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

Abstract

Mathematical models are described which provide an improved understanding of the interaction with biological objects of electromagnetic energy in the radio frequency-microwave spectrum. Significant dosimetric data are derived for the absorption characteristics and internal dose distribution, using a multi-layered sphere model exposed to plane wave radiation over the frequency range 0.1 to 10 GHz. Using such data, some generalized conclusions are presented which provide useful dosage estimation methods to those involved in the health effects of nonionizing radiation research.

Introduction

There is increasing concern regarding the potentially harmful effects of exposure to nonionizing electromagnetic radiation in the radio frequency (RF) - microwave spectrum (wavelengths range of approx. 3000 to 0.1 cms). Such concerns have been prompted by two factors: the increasing proliferation of high-powered RF and microwave sources, such as radio and TV broadcast transmitters, radar transmitters, domestic and industrial cooking and drying ovens, diathermy devices, etc., leading to the potential for excessive human exposure to man-made radiation. The other factor is the thousand fold difference which now exists between the ANSI recommended protection guide of 10 mW/cm^2 maximum exposure rate in the United States and the more conservative protection standard adopted in the Soviet Union and Eastern Europe (exposures greater than 2 hours). Much research has been done in this country on the short-term, high level heating effects of microwave energy. This work has been well documented in a number of recent review papers.[1,2,3] Work on the chronic effects of long term, low level exposure has been pursued by Soviet workers for many years and is now being strongly emphasized in this country.[4] Findings are frequently contradictory and often not repeatable, leading to much controversy and speculation regarding the effects of low level exposure. This is undoubtedly due, in large part, to the difficulties involved in measuring or estimating absorbed energy dose for the subject undergoing irradiation.

Johnson[5,6] has emphasized that observed biological effects or phenomena can only be related to the absorbed dose and not to the incident power density. The degree to which electromagnetic energy is coupled into the irradiated subject is a very complex function of size, shape, dielectric composition and orientation of the subject as well as the wavelength, spatial characteristics and polarization of the incident radiation. Furthermore, the internal distribution of absorbed energy is never uniform, except when the incident wavelength is much larger than object size, and is frequently concentrated into localized "hot spot" regions. This means that for the same exposure conditions the absorbed dose and internal dose distribution for a small object such as an experimental animal will be very different from that for a much larger object such as a human.

Because of the general complexity of the electromagnetic interaction problem, much use has been made of very simplified mathematical models in order to obtain a better understanding of the nature of this interaction. Such models consist of objects having a simple planar, spherical or cylindrical shape that are generally exposed to the simplest form of radiation; i.e., the electromagnetic plane wave. These objects are composed of various layers of homogeneous and dissipative dielectrics which approximate the known dielectric properties of various biological tissues such as muscle, fat, bone, skin, etc. Solutions for the planar model are very simple[5,7] but the results are not really applicable to any closed object with curved boundaries except when the incident wave length is very short compared to object size. The sphere model[5,7,8,9,11] has been popular because it better approximates a curved object and because the solution is well known and can be readily handled using high speed machine techniques. Such a model can be considered to be a crude representation of animal and human heads, but the analogy is obviously approximate and very limited. Some work has also been done on the interaction of cylindrical and spherical models with the more complex radiation from a direct-contact aperture source.[10,11] Models of prolate spheroid and ellipsoid shape which better approximate the characteristically elongated bodies of laboratory animals as well as humans, are presently being investigated. To date, solutions have only been obtained for the case where incident wavelength is much greater than object size.[12] The results have underlined the important dependency of energy absorption on object orientation with respect to the polarization of the incident electric field. Several workers[13] are presently attempting to solve problems involving models of arbitrary shape and homogeneity, using finite element methods and numerical solutions, but such methods are relatively costly and limited by the total number of elements that a computer can handle.

Detailed results for the multi-layered sphere model exposed to plane wave radiation are now presented. Some results for the prolate spheroid[12] are also included.

Formulation of Sphere Model Problem

Figure 1 shows the six-layered model used in this study, with a plane wave, polarized in the x-direction and propagating in the z-direction, incident upon it.

The outer most region (p = 7) or sixth layer represents air. The dielectric properties and layer thickness of the remaining regions (p = 1,2,3,4,5,6), consisting of a core of brain-like matter and five concentric layers, are summarized in Table 1 for three different sized spheres (6.6, 12 and 20 cms diameter).

TABLE 1

Region (P)	Tissue Modeled	Electrical Properties of Tissue at 10^9 Hz		Core Size and Layer Thickness, cms		
		Relative Permittivity	Conductivity $(\text{ohm-m})^{-1}$	Outer Radius r_6 = 3.3cms	6cms	10cms
1	Brain	60	0.9	r_1=2.68	r_1=5.27	r_1=9.10
2	CSF	76	1.7	0.2	0.2	0.2
3	Dura	45	1.0	0.05	0.05	0.05
4	Bone	8.5	0.11	0.2	0.28	0.4
5	Fat	5.5	0.08	0.07	0.1	0.15
6	Skin	45	1.0	0.1	0.1	0.1

Tissue electical properties were obtained from values published by Schwan[7] and others[5]. Variations of ±30% or more can exist in the figures quoted. The changes of electrical characteristics with frequency are significant and were incorporated into all aspects of this work; sets of curves giving average permittivity and conductivity changes with frequency for the various tissues modeled, were prepared and stored in a data bank.

Expansion of the incident and secondary (scattered and internally induced) fields into vector spherical harmonics is based on Stratton's formulation[8] (See Fig 1). Tangential components of E and H-fields

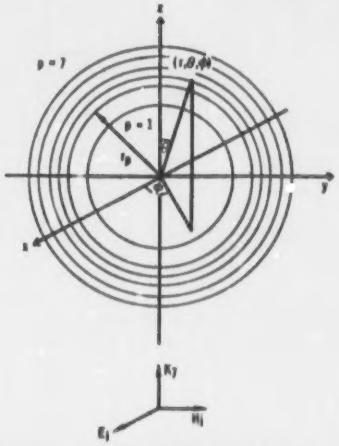

Fig. 1. Plane wave incident upon spherical model with six concentric shells.

Spherical Harmonic Expansions for Electric Fields

Incident:

$$E_i = E_0 e^{-i\omega t} \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} (m^{(1)}_{o1n} - i n^{(1)}_{e1n}).$$

Reflected:

$$E_r = E_0 e^{-i\omega t} \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} (a^r_n m^{(3)}_{o1n} - i b^r_n n^{(3)}_{e1n}).$$

Induced within sphere:

$$E_t = E_0 e^{-i\omega t} \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} (a^t_n m^{(1)}_{o1n} - i b^t_n n^{(1)}_{e1n}).$$

Scattering cross section:

$$Q_s = \frac{2\pi}{k_2^2} \sum_{n=1}^{\infty} (2n+1) (|a^r_n|^2 + |b^r_n|^2).$$

Total cross section:

$$Q_t = \frac{2\pi}{k_2^2} \mathrm{Re} \sum_{n=1}^{\infty} (2n+1) (a^r_n + b^r_n).$$

Absorption cross section, $Q_a = Q_t - Q_s$.

are then equated at the six regional boundaries in order to determine the unknown expansion coefficients.

Absorption Properties and Dose Distribution

For a simple object having a well known geometric cross-section, such as a sphere, the absorption characteristics are conveniently defined in terms of an absorption coefficient, given by the actual absorption cross section, Q_a divided by the shadow cross section. This coefficient is a measure of how efficiently the incident energy is coupled into the object being irradiated. In the contour plot of Fig 2, the absorption characteristics for different sized spheres ranging from 2 to 12.5 cms outer radii are shown in terms of the frequency of incident radiation over the spectral range 100 to 10,000 MHz (λ = 300 to 3 cms). This representation readily shows that combination of model size and incident frequency for which the energy absorption is greatest. Two major "ridge" lines running diagonally across the plot are clearly identifiable; these represent regions of resonant absorption. The third ridge line to the right of the plot represents a resonant coupling of energy into the core of the model by the outer tissue layers. Note that the absorption coefficient can considerably exceed unity in the resonant absorption regions.

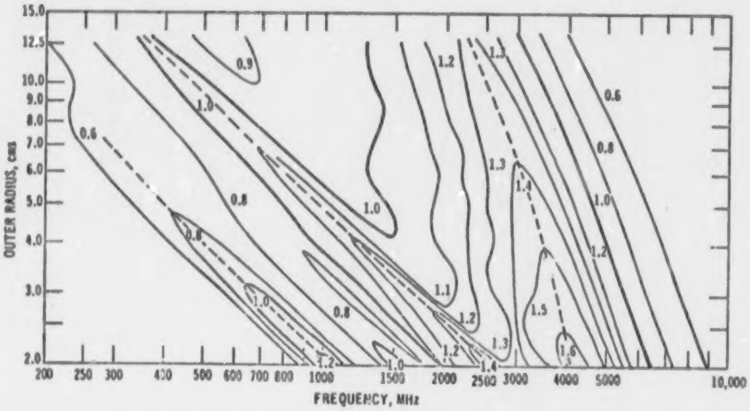

Fig. 2. Radius versus frequency diagram for multilayered sphere; the contours represent lines of constant absorption coefficient.

The internal distribution of absorbed energy (dose) in the brain-like core of a 6 cms radius sphere (roughly equivalent to infant sized head) is illustrated in Figs 3 and 4 for two different frequencies. The distributions are shown in the plane (ϕ = 0) of the incident electric field vector (E-plane) and the contours are normalized iso-dose rate lines (constant absorbed dose rate, normalized to E_0 = 1 volt/meter peak). At the resonant absorption frequency of 800 MHz (see Fig 3), a major "hot spot" concentration is found to exist immediately in front of the sphere center, due to focusing of energy into the center, as well as standing wave effects. The greatest internal field concentration was found to exist at 1650 MHz (see Fig 4) where the original hot spot has now split into two separate and more intense concentrations that are located behind the sphere center on both sides of the z-axis. At still higher frequencies microwave energy is decreasingly able to penetrate very far into the sphere owing to the greatly increased conductivity values of the core dielectric (conductivity at 3 GHz has increased three fold over its value at 100 MHz). Consequently most of the incident energy is now deposited in the front hemisphere and the internal concentrations collapse. By programming the computer to methodically scan throughout the E-plane of the model and to select the maximum field strength both inside and on the surface of the sphere, comprehensive data are obtained for both peak and average absorbed dose rates. Fig 5 shows such data as a function of frequency for the 6 cms radius sphere exposed to an incident power density of 10 mW/cm^2. At low frequencies (<500 MHz), absorption is relatively poor and the internal distribution is seen to be relatively even. In the resonant region (500-2500 MHz), absorption is strong and most of the energy is internally deposited. At frequencies above 2500 MHz, surface heating strongly predominates and the overall absorption gradually diminishes with frequency. Similar data were obtained for both a smaller (3.3 cms radius and a larger (10 cms radius) sphere, equivalent to a monkey and a human head respectively.

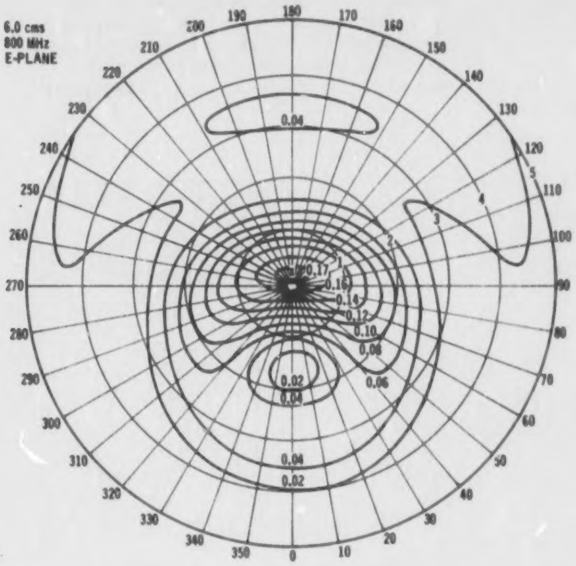

Fig. 3. Normalized dose rate distribution in core of 6 cms radius sphere at 800 MHz, E-plane.

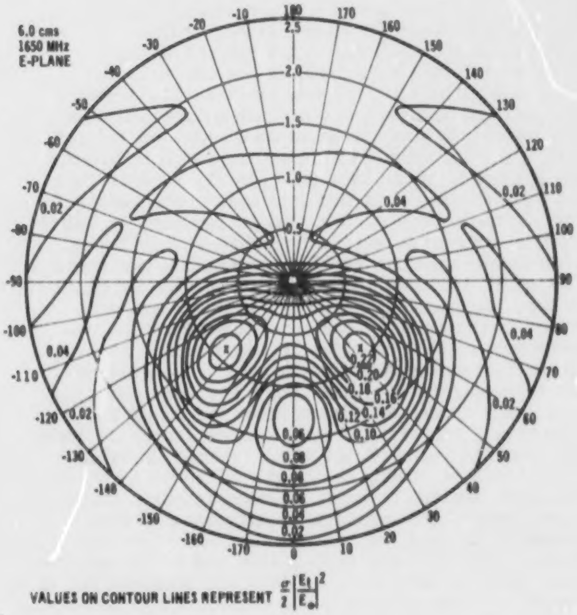

Fig. 4. E-plane distribution in core of 6 cms radius sphere at 1650 MHz.

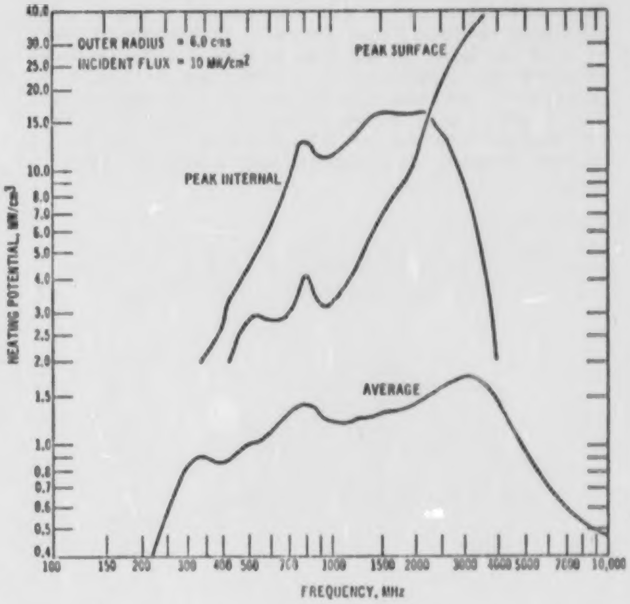

Fig. 5. Average and peak (localized) absorbed dose rate versus incident frequency for 6 cms radius sphere.

Prolate Spheroid Model

Problems involving the interaction of plane wave radiation with prolate spheriod and ellipsoid models have recently received some attention. Solutions have, so far, only been obtained for the below-resonance approximation where incident wavelength is still much longer than the model dimensions. Durney et al.[12] have obtained data on the absorption characteristics of a large man-size prolate spheriod, composed of muscle-equivalent dielectric, exposed to relatively low frequency radiation in the 1-30 MHz band. These results have shown a significant dependency of energy absorption on the orientation of the spheroid with respect to the polarization of the incident field. Durney's results are reproduced in Figs 6 and 7; maximum absorption is seen to occur for the electric polarization case when the major axis of the spheriod (length 2a) is oriented parallel to the electric field vector (see Fig 6). For the two other polarization cases, when the major axis is oriented parallel to either the magnetic field vector or along the direction of propagation (cross polarization), absorption is seen to be less than that for an equivalent sphere model of the same volume. In Fig 7, total absorption of a constant volume spheriod, normalized with respect to that of the equivalent sphere model is plotted against the eccentricity a/b of the spheriod. The orientational effects are seen to be further accentuated as the spheriod eccentricity increases; note that for the electric polarization case, energy absorption has increased to a level some seven times greater than that for the sphere model.

Solutions for the prolate spheroid problem in the resonant region, where absorption is greatest, are now being attempted. Preliminary results have shown that a man-size model will exhibit resonant absorption, under free-space conditions, in the frequency range 65-75 MHz.

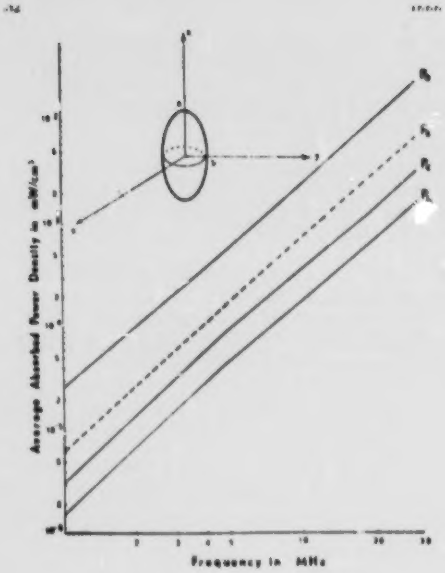

Fig. 6. Average absorbed dose rate of a muscle-equivalent prolate spheroid for three different polarizations, electric P_e, magnetic P_h and cross P_c; incident power density = 1 mW/cm², spheroid volume = 0.07 m³, a = 1 m, a/b = 7.73. The dotted line labeled P_s represents the absorption by an equivalent sphere of equal volume.
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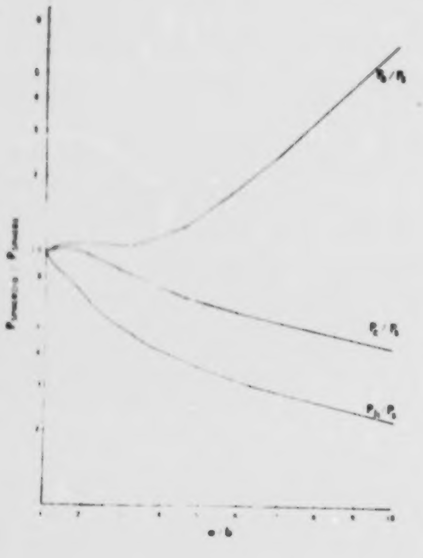

Fig. 7. Total power absorbed by an 0.07 m^3 muscle equivalent prolate spheroid, relative to that absorbed by a sphere of equal volume, versus spheroid eccentricity a/b for the three basic polarizations considered.
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Conclusions

Using the various model data, it is possible to draw some generalized conclusions regarding the interaction of microwaves with biological objects: a) All objects exhibit a resonant behavior, marked by a significant increase in absorbed energy when the incident wavelength is comparable to the object dimensions. Large objects respond uniformly to a broad spectrum of relatively low frequencies while small objects have a narrow and more peaked response at higher frequencies. The response of a specific subject will obviously depend on the subject's anthropomorphic form as well as the other factors already mentioned. b) For larger objects, where path lengths are relatively long, hot spot effects are not significant and at low frequencies the deposited energy is relatively evenly distributed. At higher frequencies virtually all the energy is frontally deposited. c) For small and medium sized objects, hot spot effects are significant over essentially the same frequency range for which resonance absorption occurs. As the object becomes smaller, peak internal fields can reach prohibitively high values at frequencies close to resonance. d) The higher the frequency, the poorer the energy penetration, so that microwaves at frequencies above about 5 GHz are incapable of penetrating even the smallest experimental object usually considered.

Finally, it is worth repeating again the conclusions reached by numerous other investigators in this field: that any effects seen during microwave exposures of experimental animals are not necessarily extrapolatable to man, owing to the widely differing absorption characteristics and internal distributions existing for man compared to that of the animal at the same frequency and same incident field level. This is clearly supported by the results of this study, which show that much greater local and average thermal burdens exist in a small object or animal than is the case for the large object (incident power density and frequency remaining the same). Great care must therefore be taken in the interpretation of results obtained during animal experimentation.

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AIR POLLUTANT HEALTH EFFECTS ESTIMATION MODEL

William C. Nelson, John H. Knelson, Victor Hasselblad
Health Effects Research Laboratory
Environmental Protection Agency
Research Triangle Park, North Carolina

Summary

A computerized system has been developed which sequentially utilizes estimates of air pollutant emissions, ambient levels, health damage functions, and populations at risk to provide an aggregate estimate of health effect. Emissions estimates should be pollutant specific for a base year (and any additional years), can be source specific such as stationary and mobile or power plant and nonpower plant, and can be geographic area specific. Ambient levels should be pollutant specific for a base year. Levels for additional years can either be provided or estimated from the emissions estimates. Arithmetic means are used to estimate chronic health effects. Geometric means and standard geometric deviations are used for acute health effects. Daily or hourly averages are estimated assuming the log normal distribution. The model can consider compound effects such as the variable short-term contribution of mobile and stationary sources. Health damage functions have been developed separately for input to the model for sulfates, photochemical oxidants, carbon monoxide, and nitrogen dioxide. Various specific health effects were considered including mortality, aggravation of asthma, acute lower respiratory disease in children, aggravation of chronic heart and lung disease in the elderly, chronic respiratory disease, and transient irritation symptoms. Age and disease status specific populations at risk were considered. Aggregate estimates were developed for each health effect and pollutant damage function. All estimates are in terms of an excess above a baseline since none of these effects are caused by air pollution alone.

Although the resulting estimates are admittedly very rough approximations, this first level of quantification is valuable for comparison of differing control strategies and for establishing ranges of uncertainty, which can be considered more fully in future research.

Introduction

Environmental control policymakers require knowledge of the complex relationships between air pollutant emissions, air quality, human exposures, and health damages for a variety of pollutant categories. This need is particularly critical for two of our largest and most important industry groups, the electric power industry and the motor vehicle transportation industry. The necessity for trade-offs is obvious as our national shortage of low-sulfur fossil fuel is superimposed on our commitment to the implementation of the Clean Air Act amendments.

Difficult decisions must be made involving consideration of benefit-cost relationships. Figure 1 shows the cyclical relationship of emissions, air quality, effects, and control decisions. The pollutants emitted by stationary sources and by motor vehicles are subjected to meteorological factors and to physical and chemical forces which produce an ambient air quality level. With knowledge of damage functions and of the exposure of a target "population," human or otherwise, one can estimate physical effects. These physical effects would include effects on human health, vegetation, animals, and materials. Policy decisions might be made on the basis of these physical effects. Our computerized model presently assumes that this is the case. In fact, the only physical effects considered to date are effects on human health.

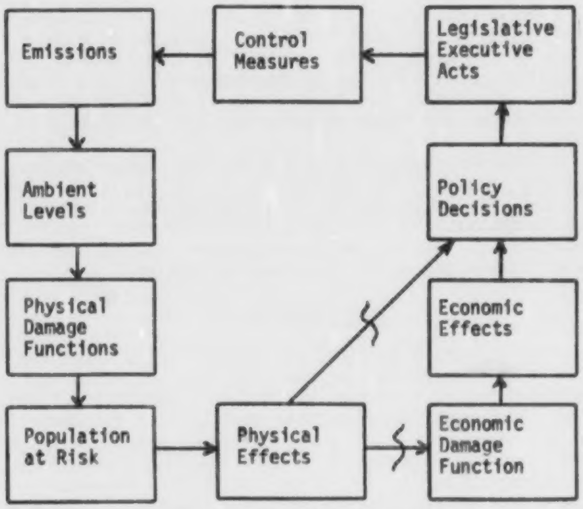

Figure 1. Schematic Relationship of Emissions, Air Quality, Effects, and Control Measures

For completeness, damage functions might also be used to estimate economic damage. A control policy must be made and enacted into law. The resulting control measures will exert their effect on emissions and the cycle shall continue.

Unfortunately, the research information base for determining these critical relationships is fragmentary rather than complete. Nevertheless, these available fragments must be utilized to provide the best possible estimates for these relationships.

This model considers the elements of Figure 1 through the physical (health) damage stage. Since the resulting estimates of health effects from various "scenario" assumptions have been presented elsewhere,[1-4] this paper will stress the methodology of the model and its flexibility as an estimation tool. The following sections describe the components of the model in some detail.

Emissions

The model requires emissions and air quality information for some base period, ideally a year. The simplest relation between emissions and air quality is based on the assumption that the change in air quality due to man-made pollution sources is proportional to the change in man-made emissions in the region of interest. Therefore if emission estimates are provided for additional years, resulting air quality for the ith year is estimated by the formula

$$(AQ_i - BAQ_i)/(AQ - BAQ) = E_i/E$$

where AQ, BAQ, and E represent total air quality, natural background air quality, and emissions for a base year, and where the subscripted variables represent these same quantities for the ith year.

It should be noted that this model assumption does not relate air quality to emissions but only relates changes in air quality to changes in emissions. This assumption provides a reasonable estimate if the meteorologic and topographic characteristics of the area and the temporal and spatial distribution of emissions remain stable over the time period of interest.

Emissions have also been classified into compartments such as mobile and stationary sources or power plant and nonpower plant sources. Various "growth" scenario assumptions can be considered for the various cases. For each, the simple assumption of a linear relation between changing emissions and air quality is made.

Emissions estimates have also been classified by geographic area. The contiguous United States has been divided into seven regions representing approximately the Northeast, the Southeast, the Eastcentral, the Midwest, the Southcentral, the Northern Plains, and the West. State boundaries have been maintained.

Air Quality

As mentioned earlier, air quality information for some base time period is required. For our model we utilized the data base of the National Aerometric Data Bank (NADB). We developed air quality data for each of the seven geographic areas mentioned previously. Additionally, each region was divided into four strata, depending on population, based on the 1970 Census. These four strata were classified as rural (including towns of less than 2500, urban places of less than 100,000, urban areas larger than 100,000 but less than 2,000,000, and urban areas larger than 2,000,000. Air quality data were derived from NADB representing each of the 28 population and geographic classes.

Obviously the inclusion of these 28 classes adds a little more realism to the model since it permits consideration of different control options for different population size areas and for different regions of the country. Additional subdivision is desirable for certain problems. For example, the south coast air basin of California was considered separately for the oxidant problem. The model can be easily modified to permit consideration of other individual regions, cities, or states.

To date, information on ambient levels has been obtained and used for suspended sulfates, oxidants, carbon monoxide, and nitrogen dioxide. More monitoring data are obviously available for some of these pollutants than for others.

The particular aerometric parameter used to estimate health damage is dependent on the type of effect. Annual arithmetic means are used to estimate health effects which are attributable to long-term pollutant exposure. Averages or maxima for shorter time periods are required for estimating acute health effects. Daily or hourly averages are calculated from the annual geometric mean and standard geometric deviation, assuming a log normal distribution. The acute health effects from these shorter exposures are aggregated so that all damage estimates are expressed on an annual basis.

Health Damage Functions

The health information base for pollutant effects was reviewed in careful detail. Although a great number of research studies have been carried out, the total information available is limited. Methodology variations in the individual studies usually prevent strict comparability of study results. The significant effects observed in many studies despite differences in the health end point, target population, and pollutants measured, ensure that pollutant effects are widespread. The data base, therefore, provides far more qualitative information than quantitative information. However, there are a relatively few pollutants and health effects for which enough reliable quantitative data exist from multiple studies to allow estimation of health damage functions.

These functions are now discussed for each relevant pollutant. Each function has been determined on the basis of excess risk of illness or death above a baseline level since none of these effects are due to air pollution alone. The specific characteristics of each function are also displayed in Table 1.

Carbon Monoxide

The effect of low-level carbon monoxide exposure on the cardiovascular system has been investigated by several investigators.[5] There is evidence from laboratory animal studies and from human volunteer studies of less severe cardiac effects,that carbon monoxide exposure can increase risk of death for individuals suffering myocardial infarctions.[6] While adverse effects might occur at very low carboxyhemoglobin levels, the damage function was constructed assuming no adverse effect could be demonstrated below a carboxyhemoglobin level of 2 percent. A linear increase in adverse effect was assumed up to a carboxyhemoglobin level of 10 percent.

There also is evidence that carbon monoxide exposure can decrease the time to onset of chest pain and increase the duration of the pain for persons with stable coronary artery disease.[7] Studies with human volunteers were conducted at 2.9 percent carboxyhemoglobin and at 4.5 percent carboxyhemoglobin. The total mean time of increased disability (decreased activity plus increased duration of chest pain) was 87 seconds at 2.9% COHb and 144 seconds at 4.5% COHb. Linear damage functions were estimated for these data points assuming an effects threshold ranging from 0.5% COHb to 2.0% COHb. The most reasonable point estimate of the threshold has been determined to be 1.5% COHb and this is the value shown in Table 1.

Suspended Sulfates

Exposure to elevated levels of sulfur oxides, particularly suspended sulfate aerosols, has been shown to cause or aggravate several health effects.[8] A problem is that these effects were observed in community studies where levels of sulfur dioxide, acid-sulfate aerosol, and suspended particulate matter were usually simultaneously elevated. Another limitation is that for some studies, suspended sulfate levels had to be estimated from measured sulfur dioxide concentrations.

Despite these difficulties, it is likely that short-term elevated exposure to sulfates is largely responsible for the perceptible increases in daily mortality observed during air pollution episodes in New York,[9,10] London,[11] and Oslo.[12] Data points from these studies were plotted and a linear regression equation was estimated. An effects threshold for a 24-hour average sulfates concentration was estimated to be 25 $\mu g/m^3$.

Elevated short-term exposures also cause aggravation of asthma and of preexisting heart and lung diseases. The studies of volunteer asthmatics were done in the United States[8] and Japan.[13] The studies of elderly volunteers with chronic heart or lung disease were done in Chicago[14] and New York.[8] Results indicated that each of these susceptible groups were more likely to experience an attack or a worsening of their chronic symptoms on high sulfate days. Data points from these studies allowed plots to be constructed and, as with the mortality data, linear regression equations to be estimated. For the asthma damage function, a threshold was estimated to occur at a daily average sulfate concentration of 6 $\mu g/m^3$ and for the aggravation of preexisting heart and lung

Table 1. Summary of Damage Function Characteristics

Pollutant and Health Effect	Population at Risk	Assumed Baseline Frequency of Disorder within Population at Risk	Pollutant Concentration Threshold For Effect	Effect Increase as % of Baseline Per Pollutant Unit Above Threshold
Carbon Monoxide				
Mortality	One-sixth of persons suffering myocardial infarctions or sudden coronary death (0.26 percent of population)	Prevalence of one out of 200 of population at risk	2.0 % COHb or 13.1 mg/m^3 8-hour average CO	5.0% per % COHb
Angina Pectoris	Two percent of the population	One attack per day lasting 254 seconds per attack or 0.07 person-hours per day	1.50% COHb or 9.5 mg/m^3 8-hour average CO	18.75% per % COHb
Oxidants				
Aggravation of Heart and Lung Disease in Elderly	The prevalence of chronic heart and lung disease among the 11 percent of the population older than 65 years is 27 percent	One out of five of population at risk complain of symptom aggravation on any given day	400 $\mu g/m^3$ for one hour or more	1.75% per 100 $\mu g/m^3$
Aggravation of Asthma	The prevalence of asthma in the general population is 3 percent	One out of 50 asthmatics experience an attack each day	400 $\mu g/m^3$ for one hour or more	1.75% per 100 $\mu g/m^3$
Eye Discomfort	Healthy Population (Excludes persons with asthma or heart and lung disease)	Five percent per day	260 $\mu g/m^3$ for one hour or more	3.25% per 100 $\mu g/m^3$
Cough	Healthy Population (Excludes persons with asthma or heart and lung disease)	Ten percent per day	400 $\mu g/m^3$ for one hour or more	1.75% per 100 $\mu g/m^3$
Chest Discomfort	Healthy Population (Excludes persons with asthma or heart and lung disease)	Two percent per day	420 $\mu g/m^3$ for one hour or more	1.0% per 100 $\mu g/m^3$
Headache	Healthy Population (Excludes persons with asthma or heart and lung disease)	Ten percent per day	100 $\mu g/m^3$ for one hour or more	.35% per 100 $\mu g/m^3$
Nitrogen Dioxide				
Lower Respiratory Disease in Children	All children in the population or 23.5 percent of population	Fifty percent of children have one attack per year	50 $\mu g/m^3$ annual average	5.0% per 25 $\mu g/m^3$
Days of Restricted Activity from Lower Respiratory Disease	Children with a lower respiratory disease	2.66 days per attack	50 $\mu g/m^3$ annual average	5.0% per 25 $\mu g/m^3$

Table 1. (Continued)

Pollutant and Health Effect	Population at Risk	Assumed Baseline Frequency of Disorder within Population at Risk	Pollutant Concentration Threshold For Effect	Effect Increase as % of Baseline Per Pollutant Unit Above Threshold
Sulfates				
Mortality	Total Population	Daily death rate of 2.58 per 100,000	25 $\mu g/m^3$ for one day or more	2.5% per 10 $\mu g/m^3$
Aggravation of Heart and Lung Disease in Elderly	Same as above for oxidants function	Same	9 $\mu g/m^3$ for one day or more	14.1% per 10 $\mu g/m^3$
Aggravation of Asthma	Same as above for oxidants function	Same	6 $\mu g/m^3$ for one day or more	33.5% per 10 $\mu g/m^3$
Lower Respiratory Disease in Children	Same as above for nitrogen dioxide function	Same	13 $\mu g/m^3$ for several years	76.9% per 10 $\mu g/m^3$
Chronic Respiratory Disease				
Nonsmokers	62 percent of population age 21 or older	Two percent prevalence	10 $\mu g/m^3$ for several years	134% per 10 $\mu g/m^3$
Smokers	38 percent of population age 21 or older	Ten percent prevalence	15 $\mu g/m^3$ for several years	73.8% per 10 $\mu g/m^3$

disease function the threshold was estimated to be 9 $\mu g/m^3$.

Long-term exposures or repeated short-term exposures to suspended sulfates have also been linked with increased acute respiratory disease in normal healthy children. Epidemiologic studies which have related observed increases in 3-year incidence rates of acute lower respiratory disease in children 12 years old and younger to increases in annual average concentrations of suspended sulfates have been carried out in the United States[8] and England.[15,16] These studies permit the estimation of a damage function.

Another health parameter linked to sulfur oxide exposure is chronic respiratory disease. Community questionnaire surveys in several United States cities[8] have consistently shown differences in prevalence of chronic respiratory disease symptoms in adults attributable to annual average exposure to suspended sulfates. In these studies, a very important codeterminant of chronic respiratory disease is individual cigarette smoking. The available data showed that cigarette smokers were slightly less affected by ambient sulfates than were their nonsmoking neighbors. The relatively large sample size of these studies made it possible to estimate a separate damage function for smokers and for nonsmokers.

Oxidants

Exposures to elevated photochemical oxidant levels have been associated with increases in minor irritation symptoms in otherwise healthy adults. A volunteer panel of student nurses in Southern California maintained daily diaries in their health symptoms.[17] Significant associations were found with daily frequency rates for headache, chest discomfort, eye irritation and cough and daily oxidant level. The investigators had estimated segmented regression lines, known as "hockey stick" functions, for each of these four health effects. The functions were used as the basis of the damage functions for our model, requiring the ordinates to be converted from observed frequency rates to percent excess above baseline frequencies.

In addition to the previously described relationships with sulfates, it is also believed that oxidants can aggravate asthma and symptoms of chronic heart and lung disease. As an estimate of a lower boundary for this functional relationship for the susceptible population at risk, the slope of the regression line for cough in a healthy population was used. As can be seen from Table 1, the baseline frequency and the target population are different for each health end point.

Nitrogen Dioxide

A damage function relating increased incidence of acute lower respiratory disease in children with annual average concentrations of nitrogen dioxide has been developed. This function and a related one estimating days of restricted activity resulting from these illnesses have been obtained from data of a study conducted in Chattanooga, Tennessee.[18] Although the survey was conducted during a period of rapidly decreasing nitrogen dioxide exposures, it is possible to form reasonable assumptions about the causes of the observed effects.[19] A regression equation was estimated for three different threshold estimates; however, the estimate providing the intermediate effect of the three appears to be most reliable and is therefore shown in Table 1. Several different estimates were also considered for the baseline annual incidence of lower respiratory disease, ranging from a per child rate of 0.5 to 2.0 attacks per year. In order to be conservative, the smallest of these, 0.5, has been incorporated into the model.

Population at Risk

As mentioned previously, the appropriate population at risk must be determined for each individual damage function and obviously will be matched as closely as possible to the target population used in the studies upon which the damage function is based. The specific populations at risk which the model considers are shown in Table 1. For each function except mortality attributable to elevated daily average sulfates, some subset of the total population is used.

The model incorporates these population subsets in two different ways. First, the specific population subsets are calculated for each of 28 population density and geographic region categories described previously in the Air Quality section. These categories are necessary for the model to determine aggregated national estimates of health impact. However, there are some situations in which national estimates are not appropriate and estimates are required for smaller regions. To provide flexibility for these situations, all population subclasses have also been calculated on the basis of a standard million population.

Health Effects

As stated in the introduction, the purpose of this paper is not to provide specific numbers for excess illnesses or premature deaths, but rather to summarize the development and methodology of the computerized model. Therefore the effects estimated, which obviously depend heavily on the region (population) and time period (air quality) of interest, will be covered only very briefly.

The magnitude of most effects is very large, if considered for an area of moderate or large population. An exception is mortality attributable to carbon monoxide for which the assumption of a threshold level of 2 percent carboxyhemoglobin (or equivalently an 8-hour average carbon monoxide level of approximately 13 mg/m^3) ensures a small estimated effect. However, for effects attributable to sulfates, the set of damage functions estimate that the annual national public health toll is on the level of millions of excess diseases and thousands of premature deaths. The estimated figures for effects attributable to oxidants and nitrogen dioxide are also very large as is the estimate of increased disability from angina pectoris attributable to carbon monoxide.

Conclusion

The fact that the national estimates of health effects attributable to air pollutant exposure are very large brings out several major points.

First, it must be stressed that the damage functions documented in this model provide very rough estimates of reality. Although these functions are believed to be the best available from the present health information base, their limitations must constantly be remembered. These functions should be frequently reevaluated and revised.

Second, the commitment to performing new research studies must be renewed. These studies must have the proper research design and methodology to permit valid quantitative results. Too often in the past, only qualitative information has been obtained of air pollution's effect on health. Also, investigators must increase their efforts to extract quantitative results from their available data by use of improved statistical analysis procedures.

Third, the existence of this computerized model at least provides a flexible mechanism for systematic assessment of the magnitude of environmentally related public health problems. Its use can aid in the specific definition of feasible alternatives and hence in the making of many of our present difficult environmental decisions.

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MORTALITY MODELS: A POLICY TOOL

Wilson B. Riggan, Ph.D., John B. Van Bruggen, Larry Truppi, Marvin Hertz, Ph.D.
Environmental Protection Agency, Research Triangle Park, N.C.

Summary

The recent Pittsburgh air pollution episode in November 1975 presents a striking need to use daily mortality models as a policy tool. In this preliminary study we found 16 deaths when the episode period was compared to the same four days of the week before, and the same four days of the week following the episode. Estimated excess deaths of 23 were found when the period of the episode was compared to the same month and period in the years 1962 through 1972. However, after fitting the model which accounted for temperature and other covariates we found only 14 deaths. In the preceding comparison the effect of temperature had been assigned to air pollution.

Mortality Models: A Policy Tool

With the great improvement in air quality monitoring technology, there is a strong accompanying need to quantify the health impact from environmental pollution. The recent Pittsburgh episode in November 1975 is a striking example of this present need. The Donora, Meuse Valley, New York, and London episodes of previous decades, which were handicapped by a lack of pollution exposure data, also provide glaring examples of this present need for more air monitoring data which can be related to observed health changes.

An important tool for improving the assessment of the total health effects of pollution is the use of daily mortality models. Although man reacts to pollution through a full spectrum of biological responses ranging from subtle physiologic changes to death, mortality is currently the best documented and defined health indicator available. It is extremely noteworthy to recall that statistically strong effects were not obvious at the time of some of the historic pollution episodes. The adverse health effects in the 1952 London episode, for example, became clear only when mortality records became vital statistics.

This paper will describe the use of daily mortality models based on single forecast equations that can apply to metropolitan areas in the Northeastern United States. Specifically the Pittsburgh pollution episode of November 17-20, 1975, will be discussed, using the model to draw mortality inferences. The models enable epidemiologists to estimate deaths caused by high concentration of air pollution. Mortality models are very useful to prospective pollution control in that they enable authorities to forecast the probable effect of a specific control action and later to assess the effectiveness of controls.

Why use a model rather than the real world? Admittedly, a model is a crude "Alice In Wonderland" simplification of the real world. But it provides information on relationships between measurable factors which may be adjusted for, or controlled. The model must be scientifically valid in that it must approximate a microcosm of the real world. The validity of various models can be compared by how closely they approximate the actual observation data.

Materials and Methodology

For the recent Pittsburgh episode we have three major sources of mortality data: National Center for Health Statistics; Department of Vital Statistics, the State of Pennsylvania, and Allegheny County Health Department. The National Oceanic and Atmospheric Administration supplied the meteorological data. Aerometric data were supplied by the Allegheny County Air Pollution Control Board.

Background of the Pittsburgh Episode

The National Weather Service Forecast Office at Pittsburgh Airport issued an Air Stagnation warning at noon, Monday, November 17, 1975. The areas covered included western Pennsylvania, several eastern Ohio and northern West Virginia counties. A large high pressure system became stationary over the State of West Virginia, causing strong surface temperature inversions which trapped cooler air at the ground, particularly in valleys such as are common around Pittsburgh. Pittsburgh's location also brought very light surface winds causing poor dispersion. Wind speeds at the Pittsburgh Airport averaged 6.8 kph on November 17, fell to 4.2 kph on November 18, 4.0 kph on November 19, and rose to 13.7 kph on November 20, the last day of the episode. Table 1 presents daily maximum and minimum temperatures, departure from normal average temperature, afternoon mixing depths, average wind speed, resultant wind direction and speed, and average relative humidity.

Table 1

Daily Weather Conditions
Nov. 17 to Nov. 20, 1975

	17	18	19	20
Temperature (C)				
Maximum	16.7	17.2	17.2	18.3
Minimum	1.7	2.2	1.7	1.7
Departure from Normal (C)	+4.4	+5.6	+5.0	+6.12
Afternoon Mixing Depth (m)	926	1,061	869	927
Average Windspeed (kph)	6.8	4.2	4.0	13.7
Resultant Wind Direction (deg)	230	270	160	160
Resultant Wind Speed (kph)	6.3	3.4	1.6	13.2
Avg. Rel. Humidity(%)	60	63	60	56

Approach

We secured death certificates from Allegheny County Health Department. We compiled mortality figures for the four days of the Pittsburgh pollution episode, and the corresponding four days in the preceding and following weeks. These records were not complete, comprising 85-90 percent of ultimate recorded deaths. This variation is due to a number of residents who died outside the county; and will be added to the county records at a later time. Table 2 gives this comparison, revealing 16 excess deaths during the episode.

Table 2

Mortality Figures From Allegheny County for the Four Days of the Pittsburgh Air Pollution Episode, and the Corresponding Four Days in the Preceding and Following Week

Deaths During Episode	Average Deaths of Individuals for Preceding and Following Week	Excess Deaths During Episode
181	163.5	17.5

Discussion

By using the same four days of the preceding and the following week as a control, we have removed the day of week. However, the last day of the corresponding four-day period of the following week was Thanksgiving which normally has the higher holiday death rate. This suggests that without the holiday the excess deaths may have been greater than 17.

We adjusted for incomplete mortality records for November 1975 in the following manner. First we checked for an annual trend and found none. We divided the average daily deaths of the 11 years of November (47.3) by the average daily deaths of November 1975 (40.4). We used this factor of 1.17 to adjust the daily deaths upward for November 1975.

Table 3 compares the average number of deaths for November 17 through 20 for years 1962 through 1972 with the deaths during the Pittsburgh episode of November 17 through 20. This comparison gives an excess of 23 deaths.

Table 3

Comparison of Deaths

Day of Month	1975	Average 1962-1972	Excess Deaths
17	60	49	11
18	52	47	5
19	47	47	0
20	54	47	7
		Total	23

Probability = .048

The above comparison has removed the seasonal effect; to be sure the day of week effect has been removed, we selected for each year Monday through Thursday of the week preceding Thanksgiving for comparing with Monday through Friday of the episode.

Table 4

Comparison of Deaths by Day of Week

Day of Week	1975 Deaths	Average 1962-1972	Excess Deaths
Monday	60	49	11
Tuesday	52	48	4
Wednesday	47	44	3
Thursday	54	49	5
		Total	23

Probability = .048

Hence, the difference is not due to the day of the week or the annual cycle.

Application of Model

Daily fluctuations in mortality rates are primarily determined by four major factors:

1. Annual cycles
2. Epidemic influenza-pneumonia
3. Temperature
4. Environmental pollution.

Annual cycles of mortality are important in determining mortality rates because the highest death rates are in the winter and the lowest in the summer. Epidemic influenza-pneumonia is important because during an epidemic, death rates rise far above those due to annual cycle. Temperature has an effect as well as the annual cycle, in that a sharp drop in temperature associated with the movement of a weather front reduces mortality. Heat waves also have an extreme effect on mortality. Environmental pollutants increase mortality, but their effects are small compared to the others except in air pollution episodes. Temperature and annual cycle may have 15 to 20 times the effect of air pollution. Environmental pollution has a significant additional effect, assessable only when the other, strong effects are adequately measured.

Application

Our first step in developing an empirical forecast model for Allegheny County was to divide the 11 years of mortality data into two periods: 5 years, 1962-1966; and 6 years, 1967-1972. The first period was used to develop the model and estimate the coefficients while the second period was used to test the model.

First, daily total mortality observations were corrected to eliminate major influenza epidemics. Next, mortality data were checked for trend, and adjustable daily mortality ratios were computed as the daily observations divided by the average of the 11 years. We estimated coefficients for the following model:

$$Y_i = a_o\, X(1)^{a_1} X(2)^{a_2} X(3)^{a_3}\, e^{a_5 t_i + a_6 t_i^2 + a_7 t_i^3}$$

where Y_i = Daily mortality ratio of observed deaths on the i^{th} day multiplied by 100 and divided by the average number of deaths per day for the 11 years.

$X(1)$ = Lagged function distributes temperature effect over 3 days (used Y_{i-1} as distributed lagged function).[1]

$e^{t_i t_i^2 t_i^3}$ = Exponential polynomial function, third power of observed maximum temperature in degrees celsius for the given day.

$X(2)$ = Observed temperature minus the average temperature for the preceding seven days.

$X(3)$ = Precipitation during the day in millimeters.

$X(4)$ = Holiday effect - Thanksgiving, Christmas, etc.

Mortality is given as "mortality ratio expected."

This standardized ratio allows direct comparison between places and times, and statements about percent change in mortality per unit change in the pollution variable.

We used 1962-1966 data to estimate a set of coefficients. We also estimated a set of coefficients using 1967-1972 data. Estimated expected deaths for 1967 through 1972 with coefficients generated from the same data gave a sum of squares of deviation from expected of 98.3. Sum of squares of deviation from expected deaths for 1967-1972 using coefficients generated from data for 1962-1966 was 98.7. Therefore, the relationship found in the first period holds for the second period.

We felt justified in using the coefficients from 1962-1966 to calculate the expected mortality ratios for November 1975. The air pollution episode was the only observable unusual condition in November 1975 that could have caused expected mortality to deviate so widely.

After adjusting deaths during the episodes and for the same days of the week in the previous and following weeks for temperature, precipitation, annual cycle, and day of week, we still show at least 14 excess deaths during the episode. There seems little possibility that this result could be due to random chance.

Aerometric Data

With aerometric data for only three weeks from seven stations, we have not in this preliminary report attempted to estimate coefficients for a dose-response function. However, Figure 1 presents graphically the results using deviations from expected deaths generated by the model which adjusted for annual cycle, temperature, etc.

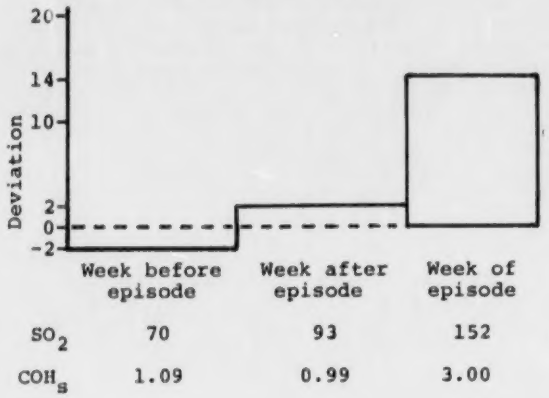

Figure 1. Comparison of Deviations from Expected Deaths Generated by the Model

The above results indicate that using deaths without considering temperature and other covariates in the Pittsburgh episode tends to inflate the number of deaths.

Comment and Conclusion

One may ask if the excess deaths would have occurred within a few days or weeks rather than during the episode. We simply do not know. However, mortality rates were higher the week following the episode than the week preceding. At least, there is no evidence that the excess deaths would have occurred during the week following the episode.

This preliminary study also found a need for more timely aerometric data, especially in pollution episodes.

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A RADIOACTIVE WASTE MANAGEMENT ASSESSMENT MODEL

S.E. Logan
Department of Chemical and Nuclear Engineering
The University of New Mexico
Albuquerque, New Mexico

S.M. Goldberg
Office of Radiation Programs
U.S. Environmental Protection Agency
Washington, D.C.

Summary

One of the major environmental concerns associated with the projected increase in nuclear power generation is the treatment and storage or disposal of high-level and transuranic radioactive waste. This model provides a detailed assessment methodology for the short-term as well as long-term quantitative effects on the environment resulting from the release of radionuclides during all phases of radioactive waste management operations. This model includes a fault tree for determination of release probabilities and their resultant magnitudes, an environmental model for calculating transport of radionuclides to man by environmental pathways and an economic model for an evaluation of associated damages. Full implementation of this technology assessment model will aid EPA and others in evaluating the radioactive high-level and transuranic waste management programs.

Background

Assessment methodology, that is both independent and flexible, is urgently needed for the evaluation of the various long-term waste disposal methods and management options.[1] High-level and transuranic radioactive waste must eventually be placed in long-term repositories for hundreds of thousands of years to prevent the entry of these wastes into the environment.[2] Management of these wastes must be accomplished in a fashion which ensures a minimum public health hazard and a minimum risk to the environment from the detrimental effects of radioactive contamination.

In this regard, a technology assessment model is being developed to perform parametric risk calculations for high-level and transuranic wastes for a variety of geologic disposal concepts, fixation processes, and reprocessing and repository operations. The model is specifically designed to translate probabilities and consequences of risk occurrences so that they can be considered in a cost-effectiveness methodology. During FY 1976, this assessment model is being utilized initially for a specific demographic and geographic site and a specific geologic concept, i.e., bedded salt in the Los Medanos area of Southeast New Mexico.[3] This model could be applied later to other specific concepts and sites that are considered or proposed by ERDA as part of their terminal storage program.

Model Development

The University of New Mexico has been developing an environmental model entitled AMRAW (Assessment Method for Radioactive Waste Management).[1] This radioactive waste management systems model has four parallel paths (Figure 1); each path represents a phase in the waste management sequence and includes a release or fault tree model, an environmental model, and an economic model. Presently, the major effort is being applied to the terminal or long-term storage branch for a site-specific environment. It is planned that the repository operations branch will be implemented during the next phase of work on the model.

The source terms for the environmental model are the quantities of the significant radionuclides that will be part of the inventory of commercial reprocessing plants and will be transported to a Federal repository. A screening method has been developed and applied to select significant radionuclides.[4] These include fission product isotopes and heavy metal isotopes. The radionuclide concentrations versus time were obtained utilizing the ORIGEN isotope generation and depletion code developed at ORNL[5] and up-to-date fuel and power conditions.[7] The waste form is assumed to be a borosilicate glass with 25 wt% waste calcine content.

Fault trees have been constructed to provide the relationships between various geologic, meteorological, and man-caused events which are potential mechanisms for release of radioactive material to the environment.[2,3,8,9] The fault tree model within AMRAW evaluates the probability for release by each of numerous potential release mechanisms (such as diapirism, tectonic process, fractures of underlying rock, groundwater transport resulting from aquifers, etc.), and the fraction of the inventory released by each such occurrence during a specific increment of time. Each path through a fault tree which leads to a release represents a set of conditions existing at a given time which together can permit a release to occur (Figure 2). Each such path comprises a "cut set" and has associated probability factors and release fractions or transfer coefficients. A flexible system has been programmed in AMRAW for the fault tree data. For each environmental release category, any number of cut sets can be accommodated, subject only to an adequate DIMENSION statement. Each cut set may consist of a number of component probability factors, which could provide a parametric survey for a single or a group of initial release conditions. Further, each component probability can be represented by any or all of the following built-in functions; constant, step change, ramp change, and exponential change. Thus, for example, the geologic process of basin-range crustal extension is expected to occur (and simultaneously represented by the code) with zero probability at the present time and gradually increasing probability ramp function in the future.

Model Application

The environmental model determines the transport to and accumulations at various receptors in the biosphere. These receptors are: air, ground surface, surface water, and groundwater (Figure 3). The model does adjust each release amount to account for environmental removal and/or fixation processes. The environmental model is also used to determine pathways from environmental input concentrations to radiation dose to man. Pathways include: immersion in air, inhalation, ingestion of groundwater, submersion in water, ingestion of contaminated food and drink, and direct surface exposure. The release increments to the four receptors in the environment are represented from all release events in the geologic condition of deep rock-melt disposal for a variety of transuranic material at several decay times (Table 1). Transfer coefficients for environmental transport and radiation dose is obtained by applying results from other available environmental codes such as Percol (groundwater transport model); INREM and EXREM (radiation dose codes); and AQUAMOD, AIRDOS, and TERMOD (environmental receptor codes).[10,11,12,13]

The economic model will calculate detailed total damage and marginal damage costs. These damages will be evaluated from the appropriate residual effects that are associated with the release of radionuclides in the waste management process. A study of relationships between long-term costs associated with radioactivity and long-term costs associated with other environmental pollutants will be started for the purpose of placing residuals effects in a proper perspective. These costs are presented in a parametric format, utilizing simplified sensitivity analysis to allow a cost-effectiveness perspective to be utilized in any decisionmaking process.

The AMRAW code is structured to allow incorporation of many of the existing or newly developed nuclear fuel cycle and environmental sciences codes as subroutines, thus allowing the main program to be as simple and straightforward as possible to avoid any "black box" mysteries. By this means, AMRAW serves as a vehicle to bring together data from several disciplines in an organized manner.

Conclusions

Application of this technology assessment model is planned by EPA for the following uses: (1) to compare and assess possible and proposed future storage and/or disposal concepts and methods for high-level waste; (2) to help develop the technical bases and guidelines for establishing environmental policy relative to the control of commercial alpha wastes and high-level wastes; (3) to apply information from the model to EPA's continuing effort to develop the generic ability to evaluate the environmental acceptability of presently operating and proposed fuel cycle facilities that produce, treat, store, and dispose of transuranic and high-level waste; and (4) to assist EPA in developing criteria and standards relating to transuranic and high-level waste management activities.

Implementation of this model is possible for a whole range of both radioactive as well as non-radioactive hazardous materials which require perpetual care. This model provides the capability to evaluate feedback effects from the results, to handle changes in any of the treatment or processing operations of these hazardous waste products, in order to minimize environmental impact. These feedback effects could serve to identify options which could act as incentives to transform these wastes into less hazardous forms, such as the application of transmutation to modify the very long-term hazard potential of transuranic wastes.

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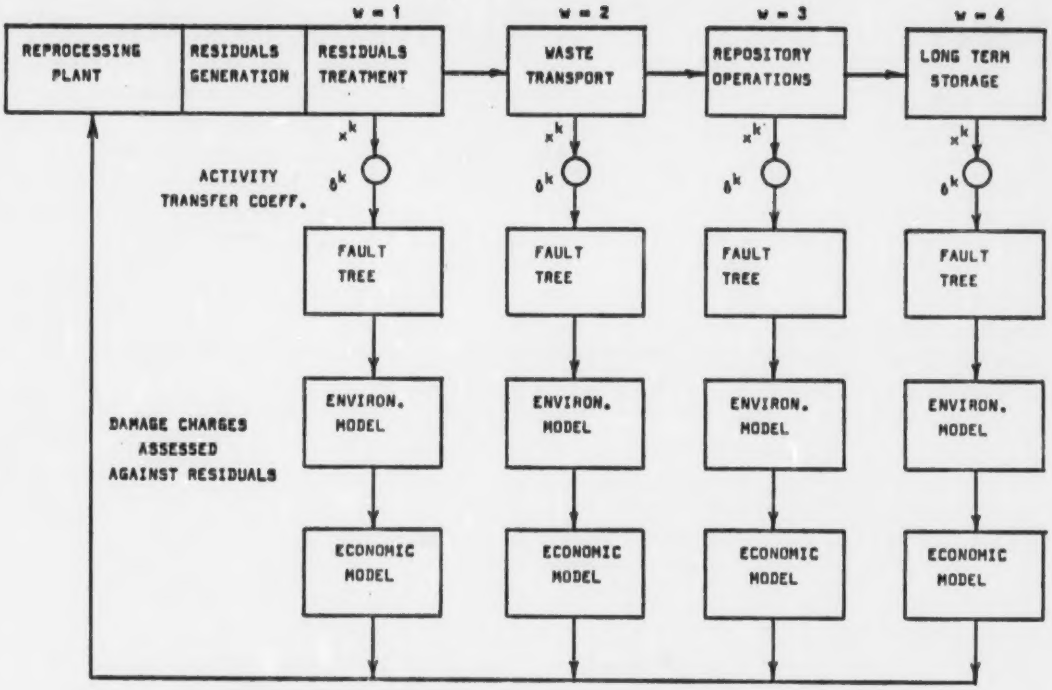
w = 1
w = 2
w = 3
w = 4
REPROCESSING PLANT
RESIDUALS GENERATION
RESIDUALS TREATMENT
WASTE TRANSPORT
REPOSITORY OPERATIONS
LONG TERM STORAGE
x^k
δ^k
ACTIVITY TRANSFER COEFF.
FAULT TREE
ENVIRON. MODEL
ECONOMIC MODEL
DAMAGE CHARGES ASSESSED AGAINST RESIDUALS

Figure 1. Radioactive Waste Management Systems Model

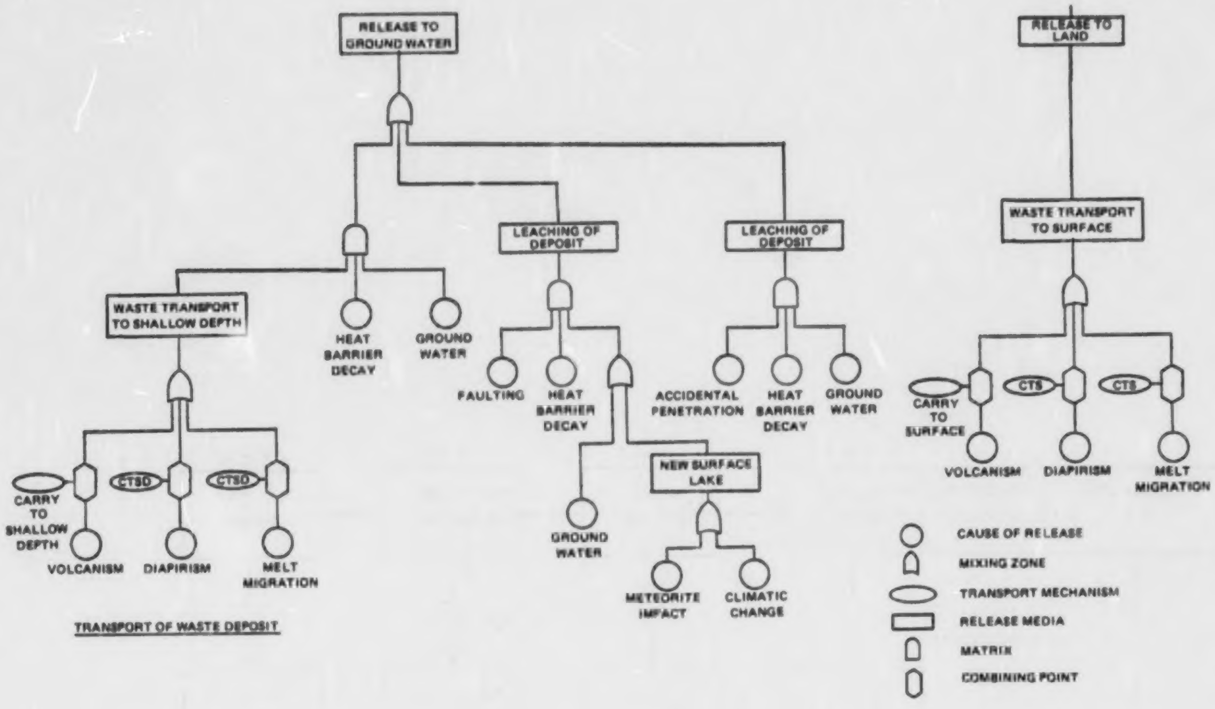
RELEASE TO GROUND WATER
RELEASE TO LAND
LEACHING OF DEPOSIT
LEACHING OF DEPOSIT
WASTE TRANSPORT TO SURFACE
WASTE TRANSPORT TO SHALLOW DEPTH
HEAT BARRIER DECAY
GROUND WATER
FAULTING
HEAT BARRIER DECAY
ACCIDENTAL PENETRATION
HEAT BARRIER DECAY
GROUND WATER
CARRY TO SURFACE
CTS
CTS
VOLCANISM
DIAPIRISM
MELT MIGRATION
NEW SURFACE LAKE
GROUND WATER
METEORITE IMPACT
CLIMATIC CHANGE
CARRY TO SHALLOW DEPTH
CTSD
CTSD
VOLCANISM
DIAPIRISM
MELT MIGRATION
TRANSPORT OF WASTE DEPOSIT
CAUSE OF RELEASE
MIXING ZONE
TRANSPORT MECHANISM
RELEASE MEDIA
MATRIX
COMBINING POINT

Figure 2. A Simplified Version of a Possible Release Cutset For Deep Rock-Melt Disposal

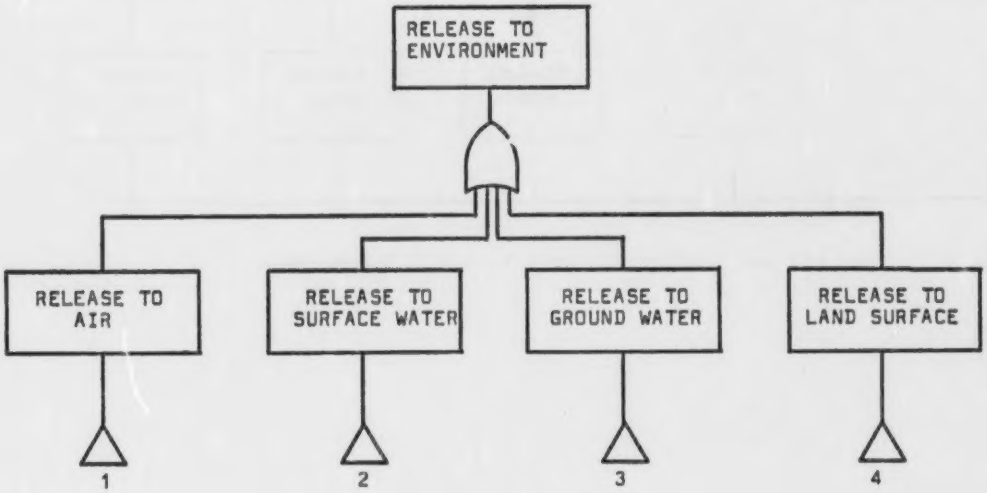
RELEASE TO ENVIRONMENT
RELEASE TO AIR
RELEASE TO SURFACE WATER
RELEASE TO GROUND WATER
RELEASE TO LAND SURFACE
1
2
3
4

Figure 3. Categorical Breakdown of Environmental Receptors in Biosphere for AMRAW

TABLE 1. Concentrations of Selected Significant Transuranic Waste Material Per Increment of Fuel for a Simulated Case of Deep-Rock Melt Disposal

TIME RECEPTOR CONCENTRATIONS (Ci)

1. RADIONUCLIDE Pu-239

TIME	AIR	GROUND SURFACE	SURFACE WATER	GROUND WATER
1.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
3.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
10.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
30.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
100.	5.51E-09	3.94E-07	5.28E-11	6.85E-12
300.	1.88E-08	1.34E-06	1.80E-10	2.34E-11
1000.	9.95E-08	7.11E-06	9.54E-10	1.24E-10
3000.	5.37E-07	3.84E-05	5.15E-09	6.68E-10
10000.	3.73E-06	2.67E-04	3.58E-08	4.64E-09
30000.	1.42E-05	1.01E-03	1.36E-07	1.76E-08
100000.	2.87E-05	2.05E-03	2.75E-07	3.57E-08
300000.	1.13E-05	8.11E-04	1.09E-07	1.41E-08
1000000.	1.36E-07	9.72E-06	1.30E-09	1.69E-10

2. RADIONUCLIDE Np-237

TIME	AIR	GROUND SURFACE	SURFACE WATER	GROUND WATER
1.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
3.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
10.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
30.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
100.	7.31E-10	5.22E-08	7.00E-12	9.08E-13
300.	2.20E-09	1.57E-07	2.11E-11	2.74E-12
1000.	8.48E-09	6.06E-07	8.13E-11	1.05E-11
3000.	2.65E-08	1.89E-06	2.54E-10	3.29E-11
10000.	9.66E-08	6.90E-06	9.26E-10	1.20E-10
30000.	2.83E-07	2.02E-05	2.71E-09	3.51E-10
100000.	9.90E-07	7.07E-05	9.49E-09	1.23E-09
300000.	2.71E-06	1.94E-04	2.60E-08	3.38E-09
1000000.	8.26E-06	5.90E-04	7.92E-08	1.03E-08

3. RADIONUCLIDE AM-243

TIME	AIR	GROUND SURFACE	SURFACE WATER	GROUND WATER
1.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
3.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
10.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
30.	0.00E-01	0.00E-01	0.00E-01	0.00E-01
100.	2.85E-07	2.04E-05	2.73E-09	3.54E-10
300.	8.06E-07	5.76E-05	7.72E-09	1.00E-09
1000.	2.71E-06	1.93E-04	2.59E-08	3.37E-09
3000.	6.87E-06	4.91E-04	6.59E-08	8.55E-09
10000.	1.68E-05	1.20E-03	1.61E-07	2.09E-08
30000.	1.93E-05	1.38E-03	1.85E-07	2.40E-08
100000.	9.47E-06	6.77E-04	9.08E-08	1.18E-08
300000.	4.71E-08	3.36E-06	4.51E-10	5.85E-11
1000000.	1.58E-10	1.13E-08	1.51E-12	1.96E-13

FOOD - AN INTERACTIVE CODE TO CALCULATE INTERNAL RADIATION DOSES FROM CONTAMINATED FOOD PRODUCTS

D. A. Baker, G. R. Hoenes and J. K. Soldat

Battelle
Pacific Northwest Laboratory
Richland, Washington 99352

Summary

An interactive code, FOOD, has been written in BASIC for the UNIVAC 1108 to facilitate calculation of internal radiation doses to man from radionuclides in food products. In the dose model, vegetation may be contaminated by either air or irrigation water containing radionuclides. The model considers two mechanisms for radionuclide contamination of vegetation: 1) direct deposition on leaves and 2) uptake from soil through the root system. The user may select up to 14 food categories with corresponding consumption rates, growing periods, and either irrigation rates or atmospheric deposition rates. These foods include various kinds of produce, grains, and animal products. At present, doses may be calculated for the total body and six internal organs from 190 radionuclides. Dose summaries can be displayed at the local terminal. Further details on percent contribution to dose by nuclide and by food type are available from an auxiliary high-speed printer. This output also includes estimated radionuclide concentrations in soil, plants, and animal products.

Introduction

The computer program FOOD is designed to calculate radiation doses to man from ingestion of foods, such as produce, milk, eggs, and meat contaminated by radionuclides. These radionuclides may be deposited on vegetation and the ground by water used for irrigation or directly from the air. A total of 14 food categories may be selected with corresponding consumption rates, growing periods, and irrigation rates or atmospheric deposition assigned by the user. At present, doses to the total body, and six internal organs from 190 radionuclides may be calculated. Dose summaries are displayed at the local terminal. Additional detains on percent contribution to dose by nuclide and by food type are available from an auxiliary high-speed printer. This latter output also includes estimated radionuclide concentrations in soil, plants, and animal products.

The program is designed to be compatible with files of releases and dose factors which are used by a program, ARRRG, which calculates doses to man from ingestion of drinking water and aquatic foods and from aquatic recreation. The program ARRRG has been described in detail previously.[1]

Model

The model presented for estimating the transfer of radionuclides (except for H-3 and C-14) from irrigation water or from air to plants through both leaves and soil to food products was derived by Soldat[2] for a study of the potential doses to people from a nuclear power complex in the year 2000.

Deposition on Food Products

The source of the radionuclide contamination of the foods may be either deposition with water used for sprinkler irrigation or deposition of airborne radionuclides. In the absence of specific data, sprinkler irrigation is normally assumed, rather than surface irrigation, because the aerial spray produced by the sprinkler leads to foliar deposition resulting in higher radionuclide concentrations in the plants (and animals consuming them) than would irrigation via furrows or drip. These latter systems can be simulated, if desired, by setting the factor for foliar retention in the program to zero.

Deposition by Irrigation Water. The deposition rate d_i from irrigation water is defined by the relation

$$d_i = C_{iw}\, I \text{ (water deposition)} \qquad (1a)$$

where:

d_i = deposition rate or flux [pCi/(m^2-d)] of radionuclide i

C_{iw} = concentration of radionuclide i in water used for irrigation (pCi/ℓ)

I = irrigation rate [ℓ/(m^2-d)]. Amount of water sprinkled on unit area of field in one day.

Deposition Directly from Air. The deposition rate onto the foliage from airborne radionuclides is defined as:

$$d_i = 86{,}400\, \bar{x}_i\, V_{di} \text{ (air deposition)} \qquad (1b)$$

where:

86,400 = dimensional conversion factor (sec/d)

V_{di} = deposition "velocity" of radionuclide i (m/sec)

$\bar{x}_i$ = annual average air concentration (pCi/m^3) of radionuclide i.

Concentration in Vegetation

The concentration of radioactive material in vegetation resulting from deposition onto the plant foliage and uptake from the soil of prior depositions on the ground is given in Equation (2).

$$C_{iv} = d_i \left[\frac{r\, T_v (1 - e^{-\lambda_{Ei} t_e})}{Y_v\, \lambda_{Ei}} + \frac{B_{iv} (1 - e^{-\lambda_i t_b})}{P\, \lambda_i} \right] e^{-\lambda_i t_h} \qquad (2)$$

where:

C_{iv} = concentration of radionuclide i in edible portion of plant v (pCi/kg)

r = fraction of deposition retained on plant (dimensionless), taken to be 0.25

T_v = factor for the translocation of externally deposited radionuclide to edible parts of plants (dimensionless). For simplicity it is taken to be independent of radionuclide and set to 1 for leafy vegetables and fresh forage, and 0.1 for all other produce, including grain. (Reference 2 lists values of this parameter which vary with nuclide.)

λ_i = radiological decay constant for radionuclide i (d^{-1})

λ_{Ei} = effective removal constant of radionuclide i from plant (d^{-1}) $\lambda_{Ei} = \lambda_i + \lambda_w$, where λ_w = weathering removal constant = 0.693/14 (d^{-1})

t_e = time of above ground exposure of crop to contamination during growing season (d)

Y_v = plant yield [kg(wet weight)/m^2]

B_{iv} = concentration factor for plant uptake of nuclide i from soil [pCi/kg(wet weight) per pCi/kg (dry soil)]

t_b = time for buildup of radionuclide in soil (d), taken to be 30 years if the source of the radionuclide is an operating nuclear facility

P = soil "surface density" [kg(dry soil)/m^2)]. Assuming a uniform mixing of all radionuclides in a plowlayer of 15 cm depth, P has a value[2] of 224 kg/m^2

t_h = holdup time (d). The time between harvest and consumption of the food.

The first term inside the brackets relates to the concentration derived from direct foliar deposition during the growing season whereas the second term relates to uptake from soil and reflects the deposition throughout the time from start of deposition until harvest of the plant.

For a cow grazing on fresh forage, t_e in Equation 2 is set equal to 30 days, the typical time for a cow to return to a particular portion of a grazing site.

Concentration in Animal Products

The radionuclide concentration in an animal product such as meat, milk, or eggs is dependent on the amount of contaminated feed or forage eaten by the animal and its intake of contaminated water. The following equation describes this calculation.[2]

$$C_{ia} = S_{ia} \left[C_{iF}\, Q_F + C_{iaw}\, Q_{aw} \right] \qquad (3)$$

where:

C_{ia} = concentration in animal product (pCi/ℓ) or (pCi/kg)

S_{ia} = transfer coefficient of radionuclide i from daily intake of animal to edible portion of animal product [pCi/ℓ (milk) per pCi/d] or [pCi/kg (animal product) per pCi/d]

C_{iF} = concentration of nuclide i in feed or forage (pCi/kg) calculated from Equation (1) above

Q_F = consumption rate of contaminated feed or forage by animal (kg/d)

C_{iaw} = concentration of nuclide i in water consumed by animals (pCi/ℓ); assumed usually to be equal to C_{iw}, and

Q_{aw} = consumption rate of contaminated water by animal (ℓ/d).

The second set of terms in the brackets in Equation (3) is omitted if the animal does not drink contaminated water. Animal consumption rates normally assumed are given in Table 1.

Values for various plant concentration factors and animal product transfer coefficients for the elements considered are given in Table 2. Plant concentration factors were taken originally from UCRL-50163, pt. IV[4] and supplemented with radionuclide data as explained in HERMES.[2] Coefficients of transfer from feed to animal products for a limited number of radionuclides were available in the literature. For those for which data were lacking comparisons were made with the behavior of chemically similar elements in man[5] and animals. In some instances, identified with an asterisk in Table 2, the value used was set to 9.9 x 10^{-4}. The most complete listing of transfer coefficients to be found is that for milk in Reference 4. The milk transfer coefficients given in this reference were intended to be maximum or "worst case" values. The authors imply, by reference to I-131, that average values would be about one-half of their listed values. As a result, the milk transfer values in Table 2 for elements lacking specific radionuclide data are one-half of those found in Reference 4.

There are some experimental data available on the transfer of several radionuclides for chicken eggs and meat.[6] Most of these literature sources were referenced in HERMES.[2,3] Unfortunately very little data is currently available on the transfer of radionuclides to beef and pork. Uncontrolled studies have been performed on the principal constituents of fallout Sr-90, I-131 and Cs-137[2] and the EPA National Environmental Research Center at Las Vegas has an ongoing study of radionuclides in cattle and milk, which hopefully, will continue to generate data usable in our model.

Tritium and Carbon-14 Model

The concentration of tritium or carbon-14 in environmental media (soil, plants and animal products) is assumed to have the same specific activity (pCi of nuclide per kg of soluble element) as the contaminating medium (air or water). The fractional content of hydrogen or carbon in a plant or animal product is then used to compute the concentration of tritium or carbon-14 in the food product under consideration. Hydrogen content in both the water and the nonwater (dry) portion of the food product is used to calculate the tritium concentration. It is assumed that plants obtain all their carbon from airborne carbon dioxide and that animals obtain all their carbon through ingestion of plants.

When carbon-14 is present only in the water used for irrigation it is difficult to model the transfer of this nuclide to vegetation, because plants acquire most of their carbon from the air. At this time we have not yet determined the transfer of carbon from the water to the air or soil. We have, therefore, conservatively assumed that plants obtain all their carbon from the irrigation water. Such an assumption could lead to plant concentrations which are high by about an order of magnitude or more. To date no operating nuclear facilities have been identified which specify releases of carbon-14 in their liquid effluents. However, this pathway could exist from migration of carbon-14 into groundwater from long-term storage of nuclear wastes..

Table 3 lists the parameters used in the computer program for tritium and carbon-14. These values may be altered based on site-specific data.

The concentration of tritium in vegetation is:

$$C_{1v} = (C_{1w})(9)(F_{hv}) \qquad (4)$$

where:

C_{1w} = concentration of tritium in the environmental water (pCi/ℓ)*

= concentration in irrigation water (for water release)

= pCi $^3H/m^3$ air ÷ absolute humidity (ℓ/m^3) (for airborne release)

1/9 = fraction of the mass of water which is hydrogen

F_{hv} = fraction of hydrogen in total vegetation (see Table 3).

The concentration of tritium in the animal product is:

$$C_{1a} = \left[\frac{C_{1F}\,Q_F + C_{1aw}\,Q_{aw}}{F_{hF}\,Q_F + Q_{aw}/9}\right] F_{ha} \qquad (5)$$

where

C_{1F} = concentration of tritium in feed or forage (pCi/kg) calculated by Equation (4) above, where now $C_{1F} = C_{1v}$

F_{hF} = fraction of hydrogen in animal feed, where now $F_{hf} = F_{hv}$ (grain)

F_{ha} = fraction of hydrogen in animal product (see Table 3)

C_{1aw} = concentration tritium in animal drinking water (set to 0 unless there is a release to water).

Similarly, the concentration of carbon-14 in vegetation is:

$$C_{3v} = C_{3w} {}^{*} F_{cv} \qquad (6)$$

where

C_{3w} = Concentration of carbon-14 in the environmental medium ÷ carbon concentration in that medium. (pCi ^{14}C/kg carbon)

= pCi ^{14}C/ℓ ÷ carbon concentration in irrigation water (kg/ℓ) for water release

= pCi $^{14}C/m^3$ ÷ carbon concentration in air (kg/m^3) for air release

F_{cv} = fraction of carbon in total vegetation.

The concentration of carbon-14 in the animal product is:

$$C_{3a} = \left[\frac{C_{3F}\,Q_F + C_{3aw}\,Q_{aw}}{F_{cF}\,Q_F + F_{cw}\,Q_{aw}}\right] F_{ca} \qquad (7)$$

For an air release $C_{3aw} = 0$ and since F_{cw} is very small compared to F_{cf}, Equation (7) reduces to:

$$C_{3a} = C_{3F}\left(\frac{F_{ca}}{F_{cF}}\right) \qquad (8)$$

Dose Calculations for Man

The dose, R_{vr}, in mrem to a person consuming vegetation is:

$$R_{vr} = \sum_{i=1}^{n} C_{iv}\,U_v\,D_{ir} \qquad (9)$$

Similarly the dose from consuming a particular animal product is:

$$R_{ar} = \sum_{i=1}^{n} C_{ia}\,U_a\,D_{ir} \qquad (10)$$

where:

U_v, U_a = annual consumption of contaminated vegetable or animal products in kg

D_{ir} = a factor which converts intake in pCi of nuclide i to dose in mrem to organ r.

Normally the exposure mode is assumed to be a 1-year chronic ingestion at a uniform rate. Dose factors are available for calculating the dose during the year of ingestion or for calculating a 50-year dose commitment. Additional factors are also available for 1- and 50-year doses from single acute intakes and for ages other than adults. However, these have not been entered into the routine program. The dose and dose commitment factors employed have been derived from the ingestion and inhalation models given in ICRP Publication 2.[5]

Dose Calculations for Biota

Since the program output lists the radionuclide concentrations in the final product from the consumption by animals of both contaminated feed and drinking water, the internal radiation dose to animals can be estimated in a manner analogous to calculation of internal dose to man. If the assumption were made that the concentration of the radionuclides in meat were similar to the average concentration in the whole animal, then the total body dose would be similar to that in the meat. The following equations can be used to calculate the dose rate in mrad/yr to an animal containing a constant concentration of a radionuclide.

$$R_c = \sum_{i=1}^{n} 18.7\,\varepsilon_{ia}\,C_{ia} \qquad (11)$$

where:

ε_{ia} = effective absorbed energy of nuclide i in the animal (MeV/dis)

18.7 = conversion factor calculated as follows:

$$(1.17 \times 10^6\ \text{dis}\cdot\text{yr}^{-1}\cdot\text{pCi}^{-1})\ (1.6 \times 10^{-5}\ \text{g}\cdot\text{mrad}\cdot\text{MeV}^{-1})$$

$$= 18.7\ \frac{\text{dis}\cdot\text{g}\cdot\text{mrad}}{\text{pCi}\cdot\text{yr}\cdot\text{MeV}}$$

C_{ia} = concentration of nuclide i in the animal (pCi/g).

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* The subscript 1 refers to tritium which is the first nuclide in the isotope listing; similarly the subscript 3 in Equation (6) refers to ^{14}C.

TABLE 1. Consumption Rates[1] of Feed and Water by Farm Animals

	Feed or Forage (kg/day) Q_F		Water (ℓ/day) Q_{aw}
Milk Cow	55	(fresh forage)	60
Beef Cattle	68	(dry feed)	50
Pig	4.2	(dry feed)	10
Poultry (chickens)	0.12	(dry feed)	0.3

TABLE 2. Plant Concentration Factors and Animal Product Transfer Coefficients

Element	Plant/Soil (Dimensionless) B_{iv}	Egg/Feed (day/kg) S_{ia}	Milk/Grass (day/ℓ) S_{ia}	Beef/Feed (day/kg) S_{ia}	Pork/Feed (day/kg) S_{ia}	Poultry/Feed (day/kg) S_{ia}
Be	4.7E-04	2.0E-02	2.0E-06	8.0E-04	1.0E-02	4.0E-01
N	7.5E+00	9.9E-04*	1.1E-02	9.9E-04	9.9E-04	9.9E-04
F	2.0E-02	9.9E-04	7.0E-03	2.0E-02	9.0E-02	9.9E-04
Na	5.0E-02	2.0E-01	4.0E-02	5.0E-02	1.0E-01	1.0E-02
P	5.0E+01	1.0E+01	1.2E-02	5.0E-02	5.4E-01	1.9E-01
Ca	4.0E-02	1.0E+00	8.0E-03	3.3E-03	3.3E-03	3.3E-03
Sc	1.1E-03	9.9E-04	2.5E-06	6.0E-03	1.0E-02	4.0E-03
Cr	2.5E-04	9.9E-04	1.1E-03	9.9E-04	9.9E-04	9.9E-04
Mn	3.0E-02	1.0E-01	1.0E-04	5.0E-03	2.0E-02	1.1E-01
Fe	4.0E-04	1.0E-01	6.0E-04	2.0E-02	5.0E-03	1.0E-03
Co	9.4E-03	1.0E-01	5.0E-04	1.0E-03	5.0E-03	1.0E-03
Ni	1.9E-02	1.0E-01	3.4E-03	1.0E-03	5.0E-03	1.0E-03
Cu	1.3E-01	2.0E-01	7.0E-03	1.0E-02	1.5E-02	2.0E-03
Zn	4.0E-01	4.0E-03	6.0E-03	5.0E-02	1.4E-01	2.0E-03
Se	1.3E+00	2.1E+00	2.3E-02	1.0E+00	4.5E-01	3.7E-01
Br	7.6E-01	1.6E+00	2.5E-02	2.0E-02	9.0E-02	4.0E-03
Rb	1.3E-01	3.0E-00	1.0E-02	1.5E-01	2.0E-01	2.0E+00
Sr	2.0E-01	4.0E-01	1.5E-03	3.0E-04	7.3E-03	9.0E-04
Y	2.5E-03	5.0E-04	5.0E-06	5.0E-03	5.0E-03	5.0E-04
Zr	1.7E-04	1.2E-03	2.5E-06	5.0E-04	1.0E-03	1.0E-04
Nb	9.4E-03	1.2E-03	1.2E-03	5.0E-04	1.0E-03	1.0E-04
Mo	1.3E-01	4.0E-01	4.0E-03	1.0E-02	2.0E-02	2.0E-03
Tc	2.5E-01	9.9E-04	1.2E-02	9.9E-04	9.9E-04	9.9E-04
Ru	1.0E-02	4.0E-03	5.0E-07	1.0E-03	5.0E-03	3.0E-04
Rh	1.3E+01	4.0E-03	5.0E-03	1.0E-03	5.0E-03	3.0E-04
Pd	5.0E+00	4.0E-03	5.0E-03	1.0E-03	5.0E-03	3.0E-04
Ag	1.5E-01	9.9E-04	2.5E-02	9.9E-04	9.9E-04	9.9E-04
Cd	3.0E-01	9.9E-04	6.2E-05	1.6E-02	1.6E-02	1.6E-02
Sn	2.5E-03	9.9E-04	1.3E-03	9.9E-04	9.9E-04	9.9E-04
Sb	1.1E-02	7.0E-02	7.5E-04	3.0E-03	7.0E-03	6.0E-03
Te	1.3E+00	4.0E-01	5.0E-04	5.0E-02	1.0E-02	1.0E-02
I	2.0E-02	1.6E+00	1.0E-02	2.0E-02	9.0E-02	4.0E-03
Cs	2.0E-03	6.0E-01	5.0E-03	3.0E-02	2.6E-01	4.5E+00
Ba	5.0E-03	4.0E-01	4.0E-04	5.0E-04	1.0E-02	5.0E-04
La	2.5E-03	2.0E-03	2.5E-06	5.0E-03	5.0E-03	4.0E-03
Ce	5.0E-04	3.0E-03	1.0E-05	1.0E-03	5.0E-03	6.0E-04
Pr	2.5E-03	4.0E-03	2.5E-06	5.0E-03	5.0E-03	1.0E-03
Nd	2.4E-03	2.0E-04	2.5E-06	5.0E-03	5.0E-03	4.0E-03
Pm	2.5E-03	7.0E-03	2.5E-06	5.0E-03	5.0E-03	1.0E-04
Sm	2.5E-03	7.0E-03	2.5E-06	5.0E-03	5.0E-03	4.0E-03
Eu	2.5E-03	7.0E-03	2.5E-06	5.0E-03	5.0E-03	4.0E-03
Tb	2.6E-03	7.0E-03	2.5E-06	5.0E-03	5.0E-03	4.0E-03
Ho	2.6E-03	7.0E-03	2.5E-06	5.0E-03	5.0E-03	4.0E-03
W	1.8E-02	9.9E-04	2.5E-04	9.9E-04	9.9E-04	9.9E-04
Pb	6.8E-02	9.9E-04	1.0E-05	9.9E-04	9.9E-04	9.9E-04
Bi	1.5E-01	9.9E-04	2.5E-04	9.9E-04	9.9E-04	9.9E-04
Po	9.0E-03	9.9E-04	1.2E-04	9.9E-04	9.9E-04	9.9E-04
Ra	1.4E-03	2.0E-05	2.0E-04	9.9E-04	9.9E-04	9.9E-04
Ac	2.5E-03	2.0E-03	2.5E-06	5.0E-03	1.0E-02	4.0E-03
Th	4.2E-03	2.0E-03	2.5E-06	5.0E-03	1.0E-02	4.0E-03
Pa	2.5E-03	2.0E-03	2.5E-06	5.0E-03	1.0E-02	4.0E-03
U	2.5E-03	3.4E-01	6.0E-04	5.0E-03	6.0E-04	1.2E-03
Np	2.5E-03	2.0E-03	2.5E-06	5.0E-03	1.0E-02	4.0E-03
Pu	2.5E-04	2.0E-03	2.5E-08	5.0E-03	1.0E-02	4.0E-03
Am	2.5E-04	2.0E-03	2.5E-06	5.0E-03	1.0E-02	4.0E-03
Cm	2.5E-03	2.0E-03	2.5E-06	5.0E-03	1.0E-02	4.0E-03
Cf	2.5E-03	2.0E-03	7.5E-07	5.0E-03	1.0E-02	4.0E-03

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* Where value unknown, a default value of 9.9E-04 was used.

TABLE 3. Calculation of Fractions of Hydrogen and Carbon in Environmental Media, Vegetation, and Animal Products

Food or Fodder	Water f_w	Carbon (dry) f_c	Hydrogen (dry) f_h	Carbon(a) (wet) F_{cv}, F_{ca}	Hydrogen(b) (wet) F_{hv}, F_{ha}
Fresh Fruits, Vegetables and Grass	0.80	0.45	0.062	0.090	0.10
Grain and Stored Animal Feed	0.12	0.45	0.062	0.40	0.068
Eggs	0.75	0.60	0.092	0.15	0.11
Milk	0.88	0.58	0.083	0.070	0.11
Beef	0.60	0.60	0.094	0.24	0.10
Pork	0.50	0.66	0.10	0.33	0.11
Poultry	0.70	0.67	0.087	0.20	0.10

Absolute Humidity ....0.008 ℓ/m^3

Concentration of carbon in water ....2.0×10^{-5} kg/ℓ(c)

Concentration of carbon in air ....1.6×10^{-4} kg/m^3(d)

(a) F_{cv} or $F_{ca} = f_c (1 - f_w)$

(b) F_{hv} or $F_{ha} = f_w/9 + f_h (1 - f_w)$

(c) Assumes a typical bicarbonate concentration of 100 mg/ℓ

(d) Assumes a typical atmospheric CO_2 concentration of 320 ppm_v.

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AIR QUALITY AND INTRA-URBAN MORTALITY

John J. Gregor
Center for the Study of Environmental Policy
The Pennsylvania State University
University Park, Pennsylvania

Summary

The effect of air pollution on white mortality for Allegheny County, Pennsylvania is examined for the years 1968-1972 through the use of eighteen weighted regressions. The mortality rates are characterized by: age (less than 45, 45-64, and 65 and over); sex (male and female); and, cause grouping (overall, pollution-related, and all other). Air pollution is demonstrated to have a greater effect on men than women in the two younger age groups and approximately the same effect on both sexes for the 65 and over age group.

The possibility that extremely high levels of air pollution can shorten lives and affect the quality of human life was painfully brought to the attention of individuals in the United States by the 1948 episode of Donora, Pennsylvania. Today few people would argue that the existence of pollution concentrations of Donora's magnitude do not have significant health effects. There is substantially less agreement, however, on the significance of the effects of smaller levels of air pollution on health.

Background

The health effects of air pollution have been given increased attention in recent years. A growing number of experimental, episodic, and epidemiological studies have shown inverse relationships between air quality and various measures of health. This paper makes use of the insights developed by these earlier works in an attempt to quantify the relationship between ambient air quality and intra-urban mortality differentials. Some of the experimental studies with animals have shown the existence of synergistic effects of sulfur dioxide (SO_2) and various types of particulates (4, 5, 10 and 21). These, and other experimental studies have shown changes in vital functions and mortality in animals, but only changes in pulmonary functions could be studied in man. For this reason, experimental studies have shed only limited light on the relationship between levels of air pollution and mortality in man.

Episodic studies conducted by Schrenk[17], Scott[18], and Wilkins[23] have shown the existence of direct relationships between high levels of air pollution and mortality. Wilkins[23] estimated that the five-day London fog of December 1952, caused at least 4,000 deaths. Similar, but not so drastic, estimates of excess mortality were also presented by Schrenk[17] concerning the 1948 Donora episode and by Scott[18] for the 1962 London episode. As can be seen from these episodic studies, they have the advantage of being able to study mortality but are hindered in that they deal only with specific episodes of abnormally high pollution. Hence, such studies are not applicable to the everyday pollution levels faced by individuals in our urban areas. As Anderson notes:

> Although the deleterious effects of acute exposures to air pollution are well established, it is not possible to extrapolate from these data to the low levels of air pollution to which persons are exposed in a modern urban society (Anderson[1] p. 585).

For these reasons, epidemiological studies have grown in popularity since, in theory, they allow one to isolate the effects of lower levels of pollution on mortality. Most of these studies have also shown an inverse relationship between air quality and mortality. The procedure usually consists of calculating different mortality rates or partial correlation coefficients for populations exposed to different air quality conditions, after controlling for socioeconomic class by dividing the area under study into four or five socioeconomic groups (Griffith[9], Winkelstein[24], and Zeidberg[25]).

There are, however, other factors which affect mortality which are correlated with air pollution. Freeman[7], for example, has shown that air quality levels of white neighborhoods are higher than those of non-white neighborhoods. These relationships have led Lave and Seskin to note:

> If the explanatory variables were orthogonal to each other, the inability to get measures on all variables would not be important. If they were independent, one could find the effect of any variable on the mortality rate by a univariate regression. However, orthogonality is not a reasonable assumption . . . This colinearity among explanatory variables means that univariate regression, or simple cross tabulations (which constitutes the preponderance of evidence), are not likely to produce results that one could interpret.
>
> (Lave and Seskin[14] p. 295).

In an attempt to circumvent these limitations, Lave and Seskin estimated their own relationships using mortality data for 117 Standard Metropolitan Statistical Areas (SMSA's) for the period 1959-1961. They used multiple regressions to explain the variance in 35 different mortality rates (characterized by age: under 28 days, under 1 year, 14 years and younger, 15-44, 45-64, and 65 and older; by race: white and non-white; and by sex: male and female). Their independent variables were minimum sulfates, mean particulates, minimum particulates, percent poor, population per square mile, percent of population 65 or older, and percent non-white, all of which do not appear in any of their specific linear regressions since only the "best" results were presented. The results of their linear regressions show a predominantly inverse relationship between mortality and ambient air quality.

Their analysis, however, was severely restricted by data limitations, the most important of these for the purpose of isolating ambient air quality's effects on mortality being the use of only one monitoring stations' readings for an entire SMSA. As they note, "it is a heroic assumption to regard these figures as representative of an entire SMSA in making comparisons across areas" (Lave and Seskin[15] p. 286).

It should also be noted that the disaggreagated mortality rates they used are probably not accurate since as Lave and Seskin note:

> These age specific death rates were derived by dividing the number of people who died by the total population. If the age distribution of people differs across cities, these approximate death rates will not even be proportional to the true rates.
>
> (Lave and Seskin [14] p. 318).

The errors in the measurement of these dependent variables could be a reason for the low coefficients of determination for their disaggregated (age, age-sex-specific) mortality rates.

Even with these limitations, Lave and Seskin have significantly advanced our insights into the epidemiological association between ambient air quality and mortality to a new peak. They have shown that after controlling for other factors which may affect mortality, air quality does exhibit a significant association with mortality. Their experiments with alternative specifications have given results not significantly different from the general linear model (Lave and Seskin[15]). Whether these associations are causal is still an unsettled question. The experimental and episodic works mentioned earlier, however, strengthen the arguments for the existence of at least an aggrevation effect.

Objectives and Significance

Recognizing the probable existence of ambient air quality's aggravation effects on mortality, it is surprising that only a few attempts have been made isolating these effects in the epidemiological laboratory. If the energy crisis continues as appears likely, this isolation will become increasingly important as primary air quality standards come under closer scrutiny; since these standards are the fundamental impediments to the use of alternative energy sources (coal and high-sulfur oil).

As noted earlier, with the exception of Lave and Seskin's work, few attempts have been made to control for the collinearity among independent variables in explaining the variance in mortality rates for areas of different air quality. However, due to data constraints, their results are subject to some debate, especially for the disaggregated mortality rates.

In an attempt to overcome these data constraints the current analysis examines long-term (1968-1972) mortality functions for small groupings of census tracts within Allegheny County, Pennsylvania. Allegheny County is particularly well suited for this type of analysis since it has neighborhoods of both good and bad air quality. Moreover, the relatively rich microcounty data base (i.e., census and air quality data) enabled the circumvention of some of the problems that beset Lave and Seskin. Specifically, the existence of a multitude of monitoring stations' readings for air quality removes reliance on a single monitoring station. The relatively accurate information of population at risk by age, sex, and race from the 1970 census ensures that the mortality rates calculated will be representative of their population even in disaggregated form.

By approaching the problem of isolating air quality's effect on mortality at the intra-urban level through the use of multiple regression analysis, it was possible to control for a majority of "other" factors which were believed to influence an individual's probability of death. This procedure allowed isolation of air quality's influence on mortality in such a way that relatively accurate shift parameters in the various mortality functions could be estimated.

The Mortality Model

Dependent Variables

Any attempt to provide a more reliable estimate of the effects of air quality on mortality, via intra-urban, cross-sectional mortality analysis, must recognize that other factors besides air quality influence the risks of death. Specifically, since many variables are collinear to air quality, it is necessary to isolate the affect of ambient air quality on mortality. The best procedure for controlling some of the most important factors is by using age-sex-race-cause-specific mortality rates. The following narrative provides a brief explanation of mortality differentials according to each classification:

Age. In general, children are not subject to the same hazards as adults. This result coupled with a decreasing ability of the body to protect itself after a certain age leads to the expectation of differentials in mortality with respect to age.

Sex. Differentials in the risk of death can also be expected on the basis of sex. Although females do experience lower mortality rates, whether or not these differentials are biological or social is still an unsettled question.

Race. Differential mortality is also exhibited by different races within any age-sex group. With the exception of those causes of death related to inherent generic deficiencies such as sickle cell anemia, this result is probably due to social class differences.

Cause. Finally, it must be recognized that air quality would be expected only to accentuate the risks of death from certain causes (bronchitis, emphysema, asthma, etc.). Therefore, deaths should be separated into various causes to enable the isolation of air quality's influence on mortality.

Thus, by controlling for age, sex and race, as well as examining cause-specific mortality rates, it is possible partially to isolate the effects of air quality on mortality. This analysis was conducted using five-year average age-sex-cause-specific mortality rates for the white population as the dependent variables in the multiple regression analysis. Another advantage of using these specific mortality rates (particularly age and sex) as dependent variables is that such variables provide valuable indicators of the primary etiological effects of air pollution. Specifically, by isolating housewives the analysis avoids complications associated with work-related pollution exposures.

Individual five-year average mortality rates were calculated by distributing the 87,349 descendants of Allegheny County during 1968-1972 to their corresponding 1970 census tract. This procedure resulted in occasional census tract groupings since place of residence was originally coded based on 1960 census tracts. Following this step, all groups were deleted for which complete census information was not available due to confidentiality suppressions. This deletion, in addition to the exclusion of individuals with no coded residence, reduced the file to 84,034 (approximately 96 percent of the original file). The remaining census tracts were then reaggregated in order to obtain a minimum of 300 deaths per area resulting in 175 groupings. It should be recognized that those groupings were constructed to minimize the variance of certain key soicoeconomic variables (i.e., family income, education, percent white) while maintaining the contiguous nature of each group.

The reason for reducing the number of areas for which mortality rates are calculated as well as using a five-year average mortality rate is that such procedures will help reduce the variance caused in these rates by small and differing sample sizes (population of the census tracts). This is an important consideration since we are concerned with the stability of these mortality rates and not their absolute size. Consider, for example, a census tract with twenty individuals, one of which dies during our five-year period. In this case the five-year average mortality rate will be 1/100 while the yearly rates will be highly unstable ranging from 1/20 to zero (undefined). This non-constant variance is also the motive for using weighted multiple regression analysis. Since these mortality rates are a proportion (or a proportion multiplied by a constant), the variance of the observed mortality rates will be σ^2/N where σ^2 is the variance of a proportion and N is the sample size. Assuming that σ^2 is appropriately the same for all samples for a given age group, then the variance of the observed mortality rates are inversely proportional to the sample size. In the weighted regression, instead of minimizing the sum of squares of errors, ΣE_i^2 where E_i is the difference between observed mortality rates and estimated mortality rates. The objective is to minimize $\Sigma E_i^2/(\sigma^2/N_i)$, which, assuming σ is constant, will be minimized when $\Sigma E_i^2 N_i$ is minimized or when $\Sigma(E_i N_i\ 1/2)^2$ is minimized. In essence, this means the errors should be weighted by a factor equal to the square root of the sample size. (See Smith, W.[20] and also Draper and Smith[6].)

Independent Variables

The rationale for using multiple regression analysis is that there exist important factors other than age, sex, race, and air quality which influence an individual's probability of death. Some of these factors may be colinear to other independent variables. These variables include income, education, social status, occupation, residence, housing, climate, availability and access to quality medical care, quantity and quality of food consumed, tobacco consumption, sanitation, and marital status (Koss[13], Shryock and Siegel[19]). Unfortunately, measurement or observation of many of these factors is extremely difficult. Certain proxies can, however, be used while estimates can be made of other variables. The following independent variables are used in the model:

Percentage of Adult White Population With High School Education. "Higher levels of education may be associated with relatively more medical care at preventive stages" (Auster, et al.,[2] p. 415). It may also be associated with the possession of better knowledge of preventive care and willingness to seek and follow a doctor's advice. In general, people with higher education also tend to have higher incomes (correlation coefficient of .83 for Allegheny County) and thus consume higher quality goods which should favorably affect their health. Due to this high colinearity only education (as opposed to education and income) is used. Negative association between education and mortality have been shown by Kitagawa and Hauser[12], Fuchs[8], and Auster, et al.[2] The estimates of this variable for each of the 175 Allegheny County groupings were taken from 1970 census data.

Total Particulates Multiplied by Sulfur Dioxide. These variables represent two of the most available air quality measurements. Although each variable was originally employed separately, the most consistent results were obtained when the measurements interacted multiplicatively. In essence, this procedure allowed for the possible synergistic effects mentioned previously. The five-year average for each of these variables was calculated from monitoring data obtained from the Allegheny County Department of Public Health. Missing values for each monitoring station were assigned the mean value for the years when such observations were available. These monitoring stations were located on a map by their USGS coordinates and, using a computerized mapping program, estimates were made for the remaining points in Allegheny County using "standard" mapping procedures. Specifically, the calculation method was a weighted average of slopes and values of nearby data points developed from a gravity-type model and modified to consider distance and direction.

The resulting interpolated values were then plotted on a map of Allegheny County to facilitate the estimation of average values of SO_2 and total particulates for each census tract grouping. A clear overlay was placed over this computer-generated map and weighted averages of the air quality variables were calculated for each census tract grouping.

Number of Days With .1 Inch or More Precipitation and Number of Days With A Maximum Temperature Less Than 32 Degrees. These variables are the two most consistent and significant of the fourteen climatological variables originally considered. Although climate has been recognized as an important factor in mortality (Hirsch[11], Petersen[16] and Berke & Wilson[3]), the literature on the cause-effect mechanism has not developed to the level where it can be a priori determined which climatological variables are of major importance. The average values for these variables were estimated using the same procedure outlined for total particulates and SO_2.

Population Per .156 Residential Acres. Proximity to other individuals can influence exposure to various diseases. This variable was calculated by dividing the total population of the area by its residential acreage.

Results

The results of applying weighted regression analysis to the white male and female five-year average mortality rates for Allegheny County are presented in Table 1. It should be recognized that the inclusion of additional independent variables for each mortality function did not significantly increase the equations overall explanatory power. The dichotomy of mortality rates into overall, pollution-related and all other is based on the a priori explanation's previously discussed. Specifically, the contention is that air quality will only influence the probability of death from certain causes (e.g., respiratory diseases) while having no discernable effect on others (e.g., motor vehicle accidents).

The interactive air quality term (Total Particulates Multiplied by SO_2) is consistently positive and significant for the pollution-related causes of death. Moreover, size of the coeffiecient increases with age, as expected, although it differs little between sexes for the 65 and above age group. For the less than 45 and 45-64 age groups the coefficient is at least twice as large for males as females, suggesting the existence of higher exposures at work.

The air quality term is negative only for the less than 45 overall and the all other causes mortality rates. Probable explanations of this result are that: 1) individuals in this age group die from non-pollution related causes, 2) the ability of the body to withstand the influence of pollution on health decrease with age, and, 3) there exists a cumulative-type influence of pollution on mortality. Since the coefficient in the overall mortality function will be, optimally, the sum of the pollution-related and all other causes coefficients, the relatively large negative sign for all other causes in the less than 45 age group also causes the overall coefficient to be negative.

The signs of the remaining coefficient are predominantly significant and of the expected sign where a priori values could be expected (percentage of adult white population with a high school education and population per .156 residential acres). For the number of days that precipitation exceeds .1 inch the sign is continually positive and significant while for number of days with a maximum temperature less that 32 degrees the sign is predominantly negative and significant.

TABLE 1. 1968-1972 White Male and Female
Age-Cause-Specific Mortality Functions

PART A - OVERALL MORTALITY FUNCTIONS[*]

Variable	Less than 45		45-64		65 and over	
	Male	Female	Male	Female	Male	Female
Percent of Adult White Population with High School Education (1)	-1.449 (5.206)[**]	-0.639 (3.041)	-14.941 (7.121)	-5.690 (5.490)	-39.621 (6.238)	-10.752 (2.047)
Total Particulates Multiplied by SO_2 (2)	-0.001 (0.327)	-0.001 (0.378)	0.045 (2.257)	0.026 (2.779)	0.112 (1.757)	0.110 (2.120)
Number of Days Precipitation > .1" (3)	2.824 (5.371)	1.713 (4.527)	19.455 (4.354)	6.996 (3.152)	111.159 (7.121)	60.013 (4.699)
Number of Days Maximum Temperature < 32 degrees (4)	-1.471 (1.368)	-1.462 (1.935)	-0.729 (0.079)	4.246 (0.943)	-49.172 (1.553)	-27.657 (1.070)
Population per .156 Residential Acres (5)	0.023 (0.773)	0.012 (0.555)	0.647 (2.733)	0.205 (1.958)	0.283 (0.471)	-0.365 (0.779)
Constant (6)	3056.927 (4.620)	2168.157 (4.622)	16862.343 (4.830)	7492.812 (4.109)	29326.868 (3.534)	31072.048 (4.467)
$\bar{R}^2$	.281	.185	.404	.404	.539	.491

[*] All mortality rates (dependent variables) are in deaths per 100,000.

[**] The values in parenthesis are the corresponding student t values.

PART B - POLLUTION RELATED CAUSE-SPECIFIC[***] MORTALITY FUNCTIONS

Variable	Less than 45		45-64		65 and over	
	Male	Female	Male	Female	Male	Female
Percent of Adult White Population with High School Education (1)	-0.406 (3.721)	-0.059 (0.651)	-9.706 (6.431)	-4.351 (6.639)	-27.284 (5.476)	-8.494 (2.123)
Total Particulates Multiplied by SO_2 (2)	0.002 (1.656)	0.001 (1.515)	0.031 (2.180)	0.014 (2.395)	0.095 (1.906)	0.097 (2.452)
Number of Days Precipitation >.1" (3)	0.271 (1.313)	0.154 (0.961)	13.494 (4.198)	3.991 (2.844)	77.549 (6.333)	43.159 (4.436)
Number of Days Maximum Temperature < 32 degrees (4)	0.606 (1.439)	-0.311 (0.971)	-2.702 (0.406)	2.777 (0.975)	-30.882 (1.243)	-20.563 (1.044)
Population per .156 Residential Acres (5)	0.004 (0.351)	0.014 (1.574)	0.338 (1.983)	0.138 (2.082)	0.015 (0.032)	-0.301 (0.843)
Constant (6)	281.944 (1.087)	697.898 (3.514)	11738.581 (4.674)	3815.604 (3.309)	19207.563 (2.956)	22439.555 (4.241)
$\bar{R}^2$	.156	.019	.348	.357	.498	.465

[***] These mortality rates are based on total deaths from tuberculosis of the respiratory system, malignant neoplasms of bruccal cavity, pharynx and respiratory system, major cardiovascular disease, acute and chronic bronchitis and bronchiolitis, emphysema and asthma.

PART C - MORTALITY FUNCTIONS - ALL OTHER CAUSES

Variable	Less than 45 Male	Less than 45 Female	45-64 Male	45-64 Female	65 and over Male	65 and over Female
Percent of Adult White Population with High School Education (1)	-1.043 (4.353)	-0.581 (3.013)	-5.236 (5.729)	-1.339 (2.289)	-12.336 (5.471)	-2.258 (1.927)
Total Particulates Multiplied by SO_2 (2)	-0.003 (1.134)	-0.002 (1.110)	0.014 (1.580)	0.012 (2.240)	0.017 (0.739)	0.013 (0.701)
Number of Days Precipitation > .1" (3)	2.553 (5.641)	1.559 (4.489)	5.960 (3.062)	3.005 (2.399)	33.610 (6.065)	16.854 (3.661)
Number of Days Maximum Temperature < 32 degrees (4)	-2.077 (2.244)	-1.151 (1.659)	1.973 (0.489)	1.469 (0.542)	-18.290 (1.627)	-7.095 (0.761)
Population per .156 Residential Acres (5)	0.019 (0.738)	-0.002 (0.122)	0.309 (2.999)	0.067 (1.137)	0.268 (1.254)	-0.064 (0.378)
Constant (6)	2774.988 (4.871)	1470.260 (3.414)	5123.750 (3.369)	3677.218 (3.574)	10119.306 (3.435)	8587.513 (3.430)
$\bar{R}^2$	.234	.193	.315	.332	.415	.360

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EVALUATION OF HEALTH DATA IN TERMS OF ENVIRONMENTAL FACTORS

Meyer Katzper
Systems and Information Analysis
Rockville, Maryland

N. Phillip Ross
Bureau of Quality Assurance, DHEW
Rockville, Maryland

Summary

Presently, improved health data is becoming available in terms of hospital records which are to be part of a national computerized data base. Simultaneously, the more comprehensive environmental monitoring which is being implemented provides measures of environmental pollutants. The question that our models address is whether stress due to environmental factors can be detected in hospital data. To the extent that hospital data reflects environmental stress, a discriminating tool is available for determining the most probably significant pollutants from a health viewpoint.

Background

A major underlying motivation for environmental studies is the recognition that environmental factors affect man's health. In carcinogenesis research, efforts have been undertaken to establish a direct link, between an environmental factor such as might exist in a special work environment and the development of cancer.[1,2] However, there have been few systematic attempts to establish a relationship between data on incidence of illness and broad-range environmental monitoring data. Epidemiological studies generally cover severe episodes of environmental pollution. In such cases, changes in morbidity and mortality patterns have been related to pollution in the community environment.[3,4] Part of the difficulty in the past of relating health and environmental factors has been a a lack of good data. Another difficulty has been insufficient realization of the practical significance of large-scale studies and a resulting lack of high-level committment to their support. These drawbacks are presently being overcome.[5,6]

This paper examines the potential use of a large-scale health data base in defining standards for levels and exposure times to environmental pollutants known to have deleterious effects on human health. In 1972, Congress passed legislation creating Professional Standards Review Organizations (PSRO). The PSRO program provides the unique opportunity to collect uniform hospital discharge records on a national basis. For the first time there will exist a comprehensive data base containing health information on an entire population. The necessity for statistical inference will be eliminated. The population data which will be available could be used to validate suspected relationships as well as to uncover relationships heretofore only hinted at in sample data sets. Once this data base is established, linkage to local and national environmental data bases will provide a new and powerful capacity for analysis of health data as it relates to environmental conditions.

In order to utilize this potential, there is a need to develop a conceptual base from which meaningful analysis of the data will be possible. Our appoach will be to develop a series of models which will present a conceptual framework on which to build more complex and realistic models enabling researchers to realize the potential of this new data base.

A series of models is considered, starting with the simplest and proceeding to introduce complicating factors. All models consider dose levels of deleterious substances and the length of time of human exposure. Within the framework of the model, we seek to answer the question of whether a response would be detectable by examination of clinical records. When results are detectable, the model presents a basis for setting human health hazard levels in terms of human health effects. As a canonical example we consider a population subjected to an ongoing environmental stressor. An attempt is made to describe possible effects of the continued stress on the population. Underlying assumptions must be made as to the characteristics of the resultant illness. These assumptions form the framework of the model which is then mathematically and logically formulated. These results can then be used to set up a quantitative methodology for establishing acceptable stressor levels. The direct and immediate benefit of the modeling is development of the methodology which will yield insight into the nature of the problem if not its actual solution.

Model Development

Background

There is no doubt that environmental pollution has adverse affects on human health. The episodes of Donora, Pennsylvania (1948) and London (1952) provide indisputable evidence that in extreme cases environmental pollution can result in considerable loss of life and in serious illness. Acute episodes of pollution represent abrupt and unusual exposure to high concentrations of pollutants, and produce the most obvious health effects. However, human populations are continually exposed to varying levels of pollutants during their lifetimes. Recent studies have shown that chronic exposure to moderate concentrations of pollutants do adversely affect human morbidity and mortality.[7]

Chronic exposure of human populations to low levels of pollutants is an inevitable consequence of man's technological development and has become a political and economic fact of life. The problem of developing standards for acceptable levels of pollutants is complex. In principle, a "dose-response" relationship can be established if the exposure levels are high and the cause and effect relationship clear; however, with low-level chronic exposure the setting of standards becomes very complex.

The models developed in this paper focus on long-term exposure of populations to low-level concentrations of environmental pollutants with known cause and effect relationships to human health. The models are simplified by design, and as stated in the introduction, are intended to provide a structural framework from which continued probing and analysis of the data will lead to more realistic models and the development of objective methodologies for the setting of standards.

In all the models discussed, the basic underlying premise is that although chemical substances are toxic at some concentration, a concentration exists for all substances from which no injurious effects will result no matter how long the exposure.[8]

Using this conceptual basis, the models are developed in such a manner as to provide for the generation of dose-response curves which will allow for estimation of standards for pollution levels based on analysis of clinical data. Even though the state-of-the-art is such that the generation of a complete set of dose-response curves for all pollutants for different types of populations is not technically feasible, the models can provide a basis for initial generation of dose-response curves which will provide the basis for decisionmaking in setting standards for individual pollutant levels in the environment.

Models

The simplest model relates effects on health to long-term chronic exposure at low levels of a single pollutant. Exposure is assumed to result in a cumulative effect over time with the resultant onset of clinical symptoms when the cumulative dose reaches a critical level. The effect may be espressed as follows:

$$Y_i = LT \quad Q = \text{Onset of Clinical Symptoms} \qquad (1)$$

where

Y_i is the cumulative effect value for the ith observation

L is the level of pollutant which is assumed to be constant over time

T is the time of continuous exposure to the pollutant

Q is the critical value for the cumulative effect.

This model assumes all individuals in the exposed population are identical in their reaction from exposure to the pollutant. The model implies a binary situation in which the ith individual does not demonstrate any clinical symptoms until the cumulative exposure effect equals or exceeds the critical value Q

$$P\ (\text{of Clinical Symptoms}) = 0 \quad \text{when } LT < Q$$
$$P\ (\text{of Clinical Symptoms}) = 1 \quad \text{when } LT \geqslant Q$$

Validation of this model required the examination of the clinical records of a cohort population (i.e., a group of individuals all exposed to level L of a pollutant at the same time for the same period of time (T)). If the model is valid, the clinical records for the cohort will show onset of symptoms for all members of the cohort at the same time. Determination of Q in turn allows for the establishment of acceptable standards for pollutant levels.

Unfortunately, humans rarely respond in such a uniform fashion as is assumed by this model. Biological variations within the cohort population will result in variations in response to constant exposure. It is not unreasonable to assume that the variations in dose-response times will be a function of biological variability resulting in the dose-response times being distributed as a random normal variate. It is possible to modify model one to accommodate this concept.

As in model one the modified model relates health effects to chronic exposure at low levels of a single pollutant; however, this model provides for individual biological variations in the members of the exposed population. This model may be expressed as follows:

$$Y_i = LT + e_i \qquad (2)$$

where

e_i = normally distributed variable representing the individual biological variability component for the ith individual. The expected value of e_i is 0.

Using this model one would expect to find in a cohort population exposed to a single pollutant at level L for a given time T (such that LT = Q) that only a portion of the cohort population would exhibit clinical symptoms as a result of exposure rather than the entire population as would be expected under model one. If we accept the assumption that e is a random variable normally distributed with an expected value of 0, then the portion of the cohort population exhibiting clinical symptoms after exposure to level L of the pollutant for time T would be one half (.50). The concept of a cumulative critical value still holds; however, each individual reacts differently to the same exposure effectively having an individualized Q level.

$$Y_i = LT + e_i$$

If LT = Q for the single pollutant, then

$$Y_i = Q + e_i$$

If $Y_i = \begin{matrix} 0 \text{ for } (Q + e_i) < Q \\ 1 \text{ for } (Q + e_i) \geqslant Q \end{matrix}$

then the sum of the Y values divided by the population size of n for a cohort population is equal to the proportion of the population exhibiting clinical symptoms. We compute the expected value of Y

$$E(Y) = E(Q + e) = E(Q) + E(e) = Q$$

Since Y is a normally distributed variable with an expected value of Q, exposure of the cohort population to LT = Q should result in 50% of the cohort exhibiting clinical symptoms of exposure to the pollutant.

The model has effectively incorporated the concept of biological variability; however, the model is reductionist in that it assumes a situation which does not occur frequently in the real world. It assumes exposure of a single cohort to a fixed level (L) of a single pollutant for a specified time (T) producing in the individual a well defined set of clinical symptoms. In general individuals are exposed to a multitude of pollutants at varying levels of concentration and for different time periods.

It has virtually been impossible in the majority of situations to isolate the clinical effects of individual pollutants, because exposure to pollution almost always involves a mixture or combination of several pollutants. The third model addresses the situation in which more than one pollutant is present and they contribute to the manifestation of a set of clinical symptoms. For the situation where there are two environmental pollutants, the model may be represented by the following equation:

$$Y_i = \alpha_1 L_1 T_1 + \alpha_2 L_2 T_2 + I + e_i \qquad (3)$$

where

Y_i = The cumulative effective value for the ith individual

α_1 = Weight factor for exposure to the first pollutant

α_2 = Weight factor for exposure to the second pollutant

L_1 = Level of concentration of first pollutant

L_2 = Level of concentration of second pollutant

T_1 = Time of exposure to first pollutant

T_2 = Time of exposure to second pollutant

I = Synergistic or antagonistic effect of interaction between the two pollutants

e_i = Measure of biological variation for ith individual

If a cohort population is exposed to constant levels of the first (L_1) and second (L_2) pollutants for a specified time (T) where

$$T = T_1 = T_2$$

such that $T(\alpha_1 L_1 + \alpha_2 L_2) = Q_{12}$

where

Q_{12} = a cumulative critical value for exposure to L_1 and L_2

then $Y_i = Q_{12} + I + e_i$

Validation of the model from clinical records becomes a matter of detecting the existence of an interactive effect. If $I = 0$, then the model is simply a linearly additive function and one would expect to detect clinical symptoms in approximately one half the cohort population after exposure to the two pollutants for time T. However, if $I \neq 0$, one must examine the data to determine the presence of synergistic or antagonistic effects due to the interactive process. For example, there have been synergistic effects observed from exposure to sulfur oxides in the presence of undifferentiated particulate matter.[9] Laboratory studies have shown that a combination of sulfur oxides and particulates may produce an effect that is greater than the sum of effects produced by the pollutants individually. The degree of potentiation is dependent on the mix of pollutants and varies across different concentration. A three-to four-fold potentiation of the irritant response to sulfur dioxide is observed in the presence of particulate matter capable of oxidizing sulfur dioxide to sulfuric acid.[10] In situations where two pollutants are involved, the validation of interactive effects through examination of clinical records is straightforward. Interactive synergistic effects would result in more than one half the cohort population exhibiting clinical symptoms after exposure to the pollutants for a time equal to T. The greater the proportion of records showing clinical symptoms, the greater the synergism. Interactive antagonistic effects would result in less than one half the cohort population exhibiting clinical symptoms after exposure to both pollutants for a time equal to T. The greater the antagonistic effect, the lower the proportion of records showing clinical symptoms.

Expansion of this model to involve more than two different pollutants is possible; however, the complications produced by the possibilities of secondary, tertiary, quaternary . . . interactions are limitless and present methodological problems of extreme complexity in relating such models to actual clinical data.

Further Modeling Consideration

In reality, individuals are exposed to a variety of pollutants at varying concentrations and for different periods of time during their lifetime. Those exposed do not necessarily suffer from a single specific pollution-induced disease, but rather experience an aggregation of clinical symptoms in part due to pollutant exposure, aggravation of a previous weakness due to prior illness, etc.

An approach to the multifactor problems of pollution-induced illness offered by the availability of clinical information on a national basis is the capability of grouping disease entities relative to the presence of environmental stressors for specified populations (populations defined by geographic groups or logical groupings). Consider a patient exposed over time to a variety of pollutants. In such a case it would be very difficult to determine which pollutant or combination of pollutants were responsible for the illness. If there is available a large accumulation of clinical and associated environmental records for different populations, it would be possible to set up a three-dimensional matrix in which we set out environmental stressors versus clinical symptoms and population. By examining the matrix it would be possible through logical elimination to determine which stressors were not related to special disease syndromes. For example, consider two populations have identical clinical symptoms and in population one, environmental stressors A and B are present and in population two environmental stressors A and C are present. It is reasonable to conclude that factor A is a critical environmental stressor in contributing to the presence of the observed clinical symptoms. Analytical techniques such as cluster analysis applied to such matrices could provide key information in relating specific pollutants or clusters of pollutants to specific disease entities in the population. Once identified, appropriate models can be developed to aid in the establishment of pollutant level standards for different populations.

The models developed in this paper do not address the complexity inherent in real-world situations. Obviously the conditions and assumptions of these models are not frequently met in real-world situations. The models are indicators of analytic approaches which must be undertaken. The basic models must be augmented and modified to accomodate the specific situation addressed by the available data. For example, one of the aspects of environmental stress that must be accounted for in evaluating health effects is the level at which permanent damage to the organism occurs. A complementary aspect of this study is the modeling of recuperation under improved conditions. A case in point is an area with good air quality which at frequent intervals gets a peak of some pollutant. The physiological effects may then be reversible; the large dose received being compensated for by the long recovery time available between peaks. These observations can form the basis for a recuperative model of environmental effects where the cumulative critical value is never reached even though exposure time exceeds that which is necessary to produce illness.

Another situation which must be addressed is the possibility that the clinical records may show stress symptoms which cannot be directly related to any given environmental stressor. Studies by Martin[11] in London showed direct relationships between levels of smoke and sulfur dioxide and respiratory and cardiac morbidity. Empirical evidence indicates that environmental stress is producing clinical symptoms in individuals with prior weaknesses. In cases where it is suspected that environmental stressors have exacerbated prior weaknesses, the extended clinical records must be examined. In some circumstances it may be desirable to carry out retrospective studies to ascertain whether environmental factors are the underlying stressors. Such studies require an extra level of data and extra inductive steps which are not presently considered by our models.

All of the models which we have discussed can be programmed and simulated. With increasing complexity when analytic formulations cannot be solved, the logical modeling structure can still be established and simulated to determine results.

Conclusion

The models which we have presented illustrate our perceptions of environmental effects and indicate how health data can provide a basis for testing of the hypotheses underlying the models. Presently, the system for gathering data is being established. With the initial gathering of data, the appropriate ranges of parameters to be used in the models will be determined. At this point, simulation will be used to indicate the effects across the empirically determined ranges. Results will be compared with data and improvement will be made as our understanding increases.

The main reason for formulation of basic models using a minimum of hypotheses and advanced techniques is that our present level of information is insufficient to support intricate theories. With the basic models as a guide, fundamental questions can be addressed and appropriate data collected for their resolution. Based on the new information obtained, the models can be revised, refined, and expanded. In this stepwise manner with the interaction of theoretical constructs with data, a firm foundation can be laid for understanding the environmental effects on health.

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INTEGRATED ASSESSMENT: CONCEPT AND LIMITATIONS

Lowell Smith, Richard H. Ball, Steve Plotkin, and Frank Princiotta
U.S. Environmental Protection Agency
Washington, D.C.
and
Peter M. Cukor
Teknekron, Inc.
Berkeley, California

Introduction

The Integrated Assessment (IA) program conducted by the Environmental Protection Agency (EPA) is a multi-agency, interdisciplinary effort to define and evaluate the various environmental and socioeconomic effects which result from energy extraction, processing, transportation, conversion and end use activities. Integrated Assessment at EPA traces its genesis to the early socioeconomic and modeling work performed within the EPA's Washington Environmental Research Center, where research was conducted on environmental assessment methodology, on environmental benefit determinations, and on linking environmental protection strategies with models of the U.S. economy.

In early 1974, following release of the Ray report (reference 1), the Office of Management and Budget established an interagency task force on "Health and Environmental Effects of Energy Use," chaired by Dr. Donald King, Department of State, and Dr. Warren Muir of the President's Council on Environmental Quality. The task force's objectives were to:

- Examine the existing Federal research program relating to the human health and environmental effects of energy use; and to
- Recommend mutually supporting multi-agency research programs, including a programmatic allocation of Federal research funds, to develop a clearer understanding of the health and environmental effects of energy use.

An important conclusion of the task force was that the social and economic consequences of alternative energy and environmental policies needed to be considered along with, and in coordination with, the health and environmental impacts of such policies. The authors of the task force report (reference 2) recommended the formation of a research program to identify "environmentally, socially, and economically acceptable (energy development) alternatives" by integrating results from the two research areas, socioeconomic and health/ecological, as well as from research on cost/benefit/risk evaluation and policy implementation alternatives. In response to these recommendations, the Office of Energy, Minerals, and Industry (OEMI) established its IA program, which is further described herein in terms of its modeling requirements.

Problem Statement

The problem addressed by the IA program is one that has become painfully apparent to society over the past several decades. The development of new technologies, or the extension of technologies to undeveloped geographical areas, carries with it a chain of impacts extending throughout the physical, economic, and social systems. Many of these impacts are initially unforeseen, yet they may have far-reaching consequences which run counter to, and even overshadow, the intended benefits brought by a technology.

The traditional research programs of the EPA have included in their analyses of energy technologies an examination of a broad range of environmental effects. This range of research effort spans the measurement of pollutants discharged from stacks, outflows, etc., determination of their ecosystem and health impacts, control technologies for controlling or mitigating these impacts, and computations of the associated control costs. The IA cuts across these several areas of research interest, emphasizing their interconnectedness for policy analysis purposes.

Additionally, the IA program attempts to carry these analyses further, by focusing on the secondary and higher order impacts of the technologies themselves and of the environmental controls applied to them. The higher order effects considered include the possible social and economic consequences of technologies on land use and population migration, and the measures of the associated impacts on: the social structure (e.g. changes from rural to urban society, influx of workers with different social values leading to conflict), the environment (e.g., influx of population creating sewage problems, destruction of natural habitats), and on the economy (e.g., demand for new construction and operation workers which may create labor shortages for previously established industry and agriculture, and capital requirements and their associated economic and environmental implications). The program also attempts to trace in depth the effects of environmental controls on the environment, society, and the economy.

An obvious prerequisite to incorporating social and economic analysis into the health and environmental effects research program is that of insuring that the more focused portions of the Federal energy research program are complete with regard to investigating in sufficient depth all of the impact areas of concern. The IA program is responsible for identifying gaps in the overall research effort that prevent a complete assessment of optimal development and environmental control alternatives. Thus, work conducted within the program consists mainly of integrative analysis rather then original research or data collection. When further original research or data collections are identified as being necessary to allow a complete analysis, the program will generally turn to the other research programs of the EPA and the other Federal agencies for assistance.

Program Objectives

The IA program is responsive to the national need of developing a well-coordinated set of energy policies which will foster the joint attainment of energy and environmental goals. Further, it provides a mechanism whereby implementation strategies for these coordinated energy policies can be conceptually tested as to their full range of socioeconomic and environmental consequences. Objectives of the IA program include:

- Identification of energy supply and conversion alternatives which are acceptable when judged jointly by environmental, social and economic criteria and constraints;
- Evaluation of the cost/risk/benefit tradeoffs of energy production, conservation, and pollution control alternatives, especially as these prevent environmental damage and secure related benefits;
- Assistance to the nation, and EPA in particular, in the selection of optimized policies for the attainment of environmental quality goals; and
- Identification of critical gaps in current energy-related research programs, and of other priority research topics, which must be addressed in order to support direct EPA responsibilities.

Program Methodology

The primary analysis tool used by the IA program is the Technology Assessment (TA). Coates (reference 3) defines TA as "the systematic study of the effects on society that may occur when a technology is introduced, extended, or modified with a special emphasis on the impacts that are unintended, indirect, and delayed." By this definition, TA precisely fits the analysis requirements defined above. The TA's incorporated in the IA program will focus on regional energy development problems and emerging energy technologies.

The appropriate way to conduct a TA remains a matter for extended debate. TA methodologies range from highly formal structures modeled by decision analysis techniques, event trees, and quantitative cost/risk/benefit analyses that stress intense interaction within one or more interdisciplinary teams. These various techniques for conducting Technology Assessments are described at length in the literature (see references 4 through 7). The IA program is deliberately neutral with respect to favoring any TA methodology, at least at this early stage of the program. This attitude is subject to change as further experience is acquired, or as special situations are encountered.

Although selection of an appropriate methodology is obviously critical, the successful conclusion of a TA may be even more closely linked to choices made regarding the scope or boundaries of the assessment. These choices are linked to:

- Identification of the decision-maker(s);
- Resources available to the assessment team; and
- Nature of the assessment subject.

For instance, local decision-makers will usually make decisions based on the impacts on their jurisdications alone. However, a TA addressed to this type of decision-maker must consider what actions outside jurisdictions might take if the client chooses a course of action which is antithetical to the interests of these outside jurisdictions. Would a state cut off financial assistance if a locality insisted on pursuing a course of action which hurt its neighbors? A TA that did not consider these aspects would be of limited value.

When the decision-maker to be addressed is the Federal Government, as is the case to a great extent within the IA program, the definition of project scope becomes quite different. The Federal decision-maker is normally placed in the rather ambiguous position of having to incorporate simultaneously the viewpoints and interests of the Nation as a whole, as well as the States and other regional or local interest groups. This type of "global" perspective can rarely be fully accommodated in a TA, and thus each assessment is forced, reluctantly, to make critical choices as to the geographical boundaries of impacts considered, the time frames to be examined, the types of impacts to be focused on, parts of fuel cycles to be stressed, etc. In multi-year assessments, such choices are particularly critical to the success of the first year efforts.

Modeling Requirements

The IA program attempts to utilize research results and specific models for relating a wide range of causes with environmental and socioeconomic effects. Some of these include:

- Source emission characterization of specified operations as a function of operating load, fuel input, etc.;
- Operating effectiveness, economic costs, effects on reliability, etc., of pollution control technologies;
- Pollutant transport within and between media;
- Pollutant chemical transformation processes which occur within a given medium;
- Pollutant uptake and concentration in food webs;
- Acute and chronic responses of organisms to pollutant exposures;
- Pollutant effects on human welfare, including as yet poorly quantifiable impacts;
- Acute and chronic human health responses to ambient pollutant concentrations;
- Economic damage expected from pollutant releases;
- Local socioeconomic effects of energy development;
- Individual, corporate and institutional response mechanisms to changes in driving forces;
- Cost/risk/benefit analysis disaggregated to specific classes of parties at interest; and
- Net energy analysis for entire fuel cycles from extraction through transportation and conversion to pollution control and waste disposal.

Results of these analyses are integrated, through the TA mechanism, into several possible cross-cuts or dimensions of comparative analysis. Of greatest interest are analyses which articulate the range of environmental and socioeconomic consequences for:

- Differing levels of pollutant control within a given energy technology;
- Alternative energy technologies within a specific geographical region;
- Selected energy technologies applied to all geographical regions; and
- Differing strategies for development of a specified energy resource, including factors such as institutional constraints, time phasing and method of extraction.

Because of their generally wide-ranging nature, which attempts to draw results from a number of disparate disciplines into a policy-oriented decision structure, the TA's within the IA program are referred to as Integrated Technology Assessments (ITA's) Each ITA attempts to integrate its results across two or more of the above listed analysis dimensions.

Current Projects

The IA program currently has two TA's fully underway, a third about to be launched, and two more in the active planning phase. The first three of these are described in some detail in order to indicate the range of modeling requirements and opportunities within the IA program.

1. An Integrated Technology Assessment of Western Energy Resource Development: The objectives of the Western Energy ITA are to:

- Assist the EPA in developing environmental control policies and implementation strategies for mitigating the adverse impacts of Western energy resource development;
- Assist EPA's Office of Research and Development in evaluating that portion of its environmental research program dealing with the problems of Western energy development;
- Provide a balanced assessment of the full range of costs and benefits stemming from alternative energy resource developments in the Western United States in order to assist Federal and State planning for such development.

This ITA is being conducted jointly by the University of Oklahoma's Science and Public Policy (S&PP) Program and the Radian Corporation. The Project Director is Dr. Irvin (Jack) White, professor of political science at Oklahoma University and assistant director of the S&PP Program.

The ITA focuses on the impacts of developing coal, oil shale, oil, natural gas, geothermal and uranium resources in 13 western states (reference 8). Development of these resources, and especially of coal and oil shale, has become a source of extreme contention among interest groups both within and outside of the region, largely because the impacts, positive and negative, are separated spatially and temporally. For example, the development will satisfy demand for energy largely in the Midwest and the Pacific coastal states, while environmental damage will largely accrue to the resource rich states inside the region. Although in the long term the overall financial position of the resource states may possibly improve from the expanded tax base created by development, short term demands for services such as education, housing, and other services associated with a rapidly expanding population will create an initial severe strain on local finances.

The Western Energy ITA team does not favor a highly structured approach to TA, and thus there is a deemphasis of formal decision analysis and cost/risk/benefit tools and model building. Impact analysis will focus on a series of site-specific and regional scenarios. Energy development levels are set by assuming levels of national energy demand based on previous forecasts and allocating shares of the supply responses to the region (possibly by utilizing the Gulf-SRI energy model). During the first year of the study, the "boundaries" can be specified as follows:

- All portions of the fuel cycle (excluding end use) are considered except that the uranium fuel cycle is examined only to the milling stage;
- The focus of attention in impact analysis will be the eight major resource states. Impacts outside the region are not considered in depth with the possible exception being at electricity demand centers in the Midwest; and
- Exogenous variables affecting development rates are not examined in depth.

The implication of these boundaries is that the ITA focuses, in the first year, on the question of how to cope with development if it occurs. The parallel questions that a "complete" TA would attempt to answer - whether or not development should occur, and how to promote the level of development desired (or, at least, how to predict the level likely to occur) - require analyses considerably beyond the first-year study boundaries.

2. An Integrated Technology Assessment of Electric Utility Energy Systems: The Electrical Utility ITA has as its objectives;

- To provide a means of testing pollution control policies and strategies which affect the electric utility industry, and which must be formulated in response to current and near terms issues.
- To identify those issues, especially environmental issues, which are likely to require policy decisions in the future, and to identify the research programs which should be initiated in order to provide a sound basis for future decisions regarding these issues.

The ITA is being conducted by the Energy and Environmental Engineering Division of Teknekron, Inc., Berkeley, California. The Principal Investigator is Dr. Peter M. Cukor; the Project Director is Mr. Glen R. Kendall.

The Electric Utility ITA focuses on the energy conversion and pollution control technology alternatives, health and ecological effects, and resultant national economic impacts associated with activities of the electrical utility industry (reference 9). Rapid depletion of the readily accessible fluid state domestic energy resources for electrical power generation, coupled with international concerns about the quantity and security of imported oil and gas, have produced a major tilt in the industry in favor of nuclear fission and coal combustion as the electricity-producing technologies of choice over the next decade. Additionally, factors such as the decreasing availability of natural gas supplies are continuing to produce a shift towards increasing electrical demand at the expense of the more traditional energy sources, even as the total national energy demand has decreased over the past two years.

The future development implied by these forces, involving development of new mining areas and increased production in established areas, development of extensive new transmission and storage facilities, construction of extremely large fossil and nuclear generating facilities, and a vast quantity of supporting development, may result in the creation of new (and the exacerbation of existing) environmental, social and economic problems that demand the close attention of the Federal government.

In contrast to the Western Energy ITA, which is considerably broader in terms of the "actors" who play significant roles in affecting the course of development, the Electric Utility ITA is structured so as to consider the actions and effects of one industry as it is affected by external forces. Thus, Teknekron's approach to conducting this ITA relies heavily on creating models to predict the behavior of the electric utility industry. These models are to be exercised towards the end of the first year by analyzing a set of scenarios which are designed to display the results on the industry, environment and society of implementing alternative policy options. A parallel effort will be conducted to critically review and analyze the data and models available to measure the impacts of alternative courses of development, and to analyze the sensitivity of current industry practices to emerging political and social changes. A particularly important part of Teknekron's work involves a thorough review of the mechanisms of atmospheric transport and transformation of sulfur oxides and their associated health impacts on human and other receptors. Currently, this area is rich with possibilities for modeling the relationship between regional sulfur oxide emissions and the adverse effects of aerosol sulfates on public health, welfare and ecological systems.

During the first year, the boundaries of the ITA are such that it will:

- Focus primarily on existing coal technologies and secondarily on other fossil fuel technologies;
- Focus on the power plant portion of the fuel cycle;
- In terms of environmental impacts focus on air pollutants and, more specifically, on long distance transport and associated chemistry of atmospheric aerosols; and
- Generally confine air impact analysis to defining exposure of populations to pollutants without calculating health effects, aesthetic or economic damages.

A description of the individual models being constructed during the first year to simulate the economic decision making practices of the utility industry and the resulting exposure of receptors to pollutant releases is contained in the following paper.

3. Ohio River Basin Energy Facility Impact Study:

Congress, in a rider to EPA's FY 76 appropriation bill has required the Office of Research and Development to conduct a study of the Lower Ohio River Basin, to "be comprehensive in scope, investigating the impacts from air, water and solid residues on the natural environment and residents of the region" which might result from an increasing concentration of power plants in the Ohio River Basin. The IA program has developed a plan for this study which casts it in the form of a regionally-focused ITA (reference 10). The scope is broadened to consider the accelerated deployment of both conventional power plants and coal-based synthetic fuel plants in the Basin, (includes portions of the states of Ohio, Illinois, Indiana, and Kentucky). The major focus will be on an in depth examination of the impacts of coal development and conversion processes on the region, its people, social infrastructure, agricultural lands and natural environments. Mechanisms to mitigate potential adverse impacts and to shape future development along environmentally and socially acceptable lines will be analyzed. Additionally, attention will be paid to extra-regional concerns, e.g., the role of Basin development in meeting national energy demands, and the issue of how much impact the long distance transport of sulfur dioxide and the resulting sulfate aerosols may have on the urbanized Northeast.

This ITA will be conducted over a two and a half year period by several teams of academic researchers who have been selected from Mid-west universities. It will be one of the most ambitious TA's yet attempted in terms of the number of separate research groups and institutions participating.

4. Other Planned Studies:

A regionally-oriented Appalachian ITA will commence in the fall of this year. It will round out the major regional ITA's which focus on accelerated coal development and utilization. A fifth ITA, to be oriented towards a thorough assessment of advanced coal combustion and conversion technologies, will begin in the early spring of 1977.

ITA studies are also planned to address pollution control issues for industries, other than primary energy producing industries. These studies will emphasize inter-industry interactions and aggregate effects of pollution from all industries. Initial methodological studies will begin in the fall of 1976.

5. Strategic Environmental Assessment System (SEAS):

Although it is not a TA in any sense, SEAS is an important enough analysis tool to merit a brief discussion here. SEAS, originally developed within the old Washington Environmental Research Center of EPA, is a system of interdependent models designed to forecast the economic, environmental and energy consequences of alternative Federal environmental policies under varying assumptions about the future. The core of SEAS is an input/output model of the United States economy (INFORUM) which models the interactions between different economic sectors.

SEAS is capable of developing estimates to 1985 of:

- Economic projections in terms of physical output for 350 industries and processes;
- Pollution control costs for 500 control technologies; and
- Projections of environmental residuals and energy use for each of 350 industries.

A detailed description of SEAS is available in reference 11.

SEAS represents a potentially important tool for technology assessment and is thus being maintained and developed further under the IA program. For instance, SEAS offers the potential to measure the national impacts of new energy development to complement the focus on in-region impacts of the regional TA's (such as the Western Energy ITA). This type of measurement is crucial if Federal decision-makers are to take into account all of the potential impacts of development alternatives.

Work currently in progress to modify SEAS includes the development of additional capability to predict energy demand in the transportation, residential and commercial, and industrial sectors. For instance, a new transportation model will forecast activity (vehicle miles traveled), emissions and energy demand, with feedbacks to the input/output model to account for changes in automobile mix and transportation efficiency.

Another important part of current work is the integration into SEAS of the Brookhaven National Laboratory's ESNS energy supply model. Addition of ESNS will allow the study of new energy sources including coal gasification and liquefaction, oil shale, off-shore oil drilling, and geothermal and solar energy. Finally, consideration is being given to extending the SEAS economic models to the year 2000, and to improving the completeness and accuracy of the regional data bases.

Although the TA is the heart of the IA program, other types of projects are undertaken in support of the general program objectives. These projects may be categorized as:

Supplementary Studies- research projects that will supplement the TA's either by providing results that will fill research gaps identified by a TA, or by providing increased coverage of issues associated with a TA, as these become identified in the course of assessment as being crucial to EPA's fulfilling its responsibilities. This category also includes integrative studies that fall short of full TA's on topics of concern to the EPA. Frequently, detailed modeling work will be funded, at it supports the direct needs of an ongoing TA. Examples of this model development might include:

- A detailed economic model of a pollution abatement technology for a specified energy conversion process, taking into account variable characteristics of input fuel types, several levels of required control, technological approach, etc.;
- Models which transform pollutant releases into ambient concentrations, especially for reactive pollutants on a regional scale; and
- A generalized model for displaying socioeconomic impacts on idealized local communities for particular energy technologies.

Integrated Assessment Methodology - projects that will develop new methods of conducting TA's and other integrative analyses. These are projects that integrate and adapt the results of research being conducted by the Office of Technology Assessment, the National Science Foundation, other Federal agencies and the private sector on TA methodology (e.g., cost/benefit/risk analysis, multivariate decision analysis, etc.) into a framework which is suitable for EPA's decision-making processes. Case studies conducted by these projects will be chosen so as to be supportive of ongoing TA's. This portion of the program includes maintenance and further development of the Strategic Environmental Assessment System (SEAS) model.

"Pass-Through Programs"- projects supporting the IA program that are conducted by other Federal agencies under EPA funding. Agencies participating in this portion of the program include USDA, TVA, ERDA, HUD, and Commerce.

Conclusions

Although the Integrated Assessment program is in its infancy, the two TA's are well enough along to have surfaced several important issues for the program. First, the TA's tend to deal with issues that go well beyond the traditional interests of the EPA. Thus, coordination with interested Federal agencies and other entities is vital not only for information exchange purposes but also to prevent questions of the "propriety" of the research from hindering its progress. Second, it has become clear that the objective of incorporating social and economic concerns into the decision-making process is extremely ambitious. Defining useful but realistic analytical boundaries is clearly one of the most crucial-if not *the* most crucial-problems facing the program. The danger here is that these boundaries may be set so wide that the level of analysis will become too shallow to be credible.

Third, a fundamental limitation to the value of policy analysis studies such as those just described is the availability of necessary inputs in the form of tested research results from the physical, biological and medical sciences, and from economics, political and the social sciences. The uncertainties are large in much of this desired information. We are limited by an ability to model many of the interactions which critically affect, or drive, policy decisions. The error bars on these uncertainties grow progressively wider as we progress in our examination of the availability of models and supporting data for pollutant releases at one end of the analysis structure through the media transport processes to consider the effect of pollutants upon distributions of receptors at the other end of the analysis structure.

Fourth, systematic methodologies to evaluate these several forms of impact within a common base of comparison are not available at present. Finally, modeling the behavior of individuals' perceptions, social structures and institutions is in an embryonic stage of development. Yet, it is these factors which, in the end, determine how we treat the environment, what economic impacts and costs are to be internalized, how much economic activity the environment must sustain. There are challenges here to engage our best efforts for some time to come.

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AN INTEGRATED TECHNOLOGY ASSESSMENT OF ELECTRIC UTILITY ENERGY SYSTEMS

Peter M. Cukor
Sanford Cohen
Glen R. Kendall
Tom L. Johnston
Teknekron, Inc.
2118 Milvia Street
Berkeley, California

Stephen J. Gage
Lowell Smith
Office of Energy, Minerals and Industry
Office of Research and Development
U.S. Environmental Protection Agency
Washington, D.C.

Introduction

Teknekron, Inc., under the sponsorship of the Office of Energy, Minerals and Industry; U.S. Environmental Protection Agency, is conducting an Integrated Technology Assessment (ITA) of Electric Utility Energy Systems. The ITA has two primary goals. The first goal is to provide EPA with the capability to assess the environmental, economic, institutional and social effects of the generation of electricity and those activities which supply the fuels used to produce electricity. These effects will be quantified for a number of scenarios. The scenario elements include alternative futures for utility development, pollution control and siting regulations. The second goal is to assist EPA in developing research and development programs whose results are necessary in order to conduct these impact assessments. The time frame for the assessments is the period 1975-2000.

The ITA is being conducted over a three-year period. The scope and direction of the first year's effort have been defined such that the results will be responsive to the key policy issues which are likely to be faced by EPA over the next 6-18 months. As a result, the first year's work emphasizes:

- Fossil fuel electricity generation
- Primary and secondary air pollutants
- Short-range and long-range dispersion of air pollutants
- Human populations exposed to air pollutants

This paper provides a description of the models, data bases and analytical techniques which are being employed in the development of the overall ITA model. This model will simulate the environmental effects associated with electricity generation and the economic impacts of alternative policies for pollution control on the utility industry and electricity consumers. It must be emphasized, however, that impact prediction is not the only product of the Integrated Technology Assessment. Rather, impact prediction provides the quantitative information which serves as input to the technology assessment exercise in which the feasibility and impact of alternative environmental policies are appraised. Thus, this paper focuses on only one part of the conceptual framework for conducting the ITA.

Modeling Methodology

The basic analytical framework for assessment of alternatives with respect to a single module of an electrical energy fuel cycle is displayed in Figure 1. Although this framework is appropriate for assessing alternative regulations for pollution control and siting for any fuel cycle module, quantification of results rests upon the assumption that such a module will actually be constructed and operated (or continued in operation, if now existing) at a definite level of production. The electric utility industry can develop in alternative ways over the coming decades. Future developments will include alternative fuel cycles, fuel cycle configurations, facility sites, pollution control technologies, regulatory policies, demand growth rates, etc. Control levels and siting limitations will affect not only production costs and environmental impacts, as indicated by Figure 1, but will also affect the decisions made within the utility industry with regard to employing or not employing these technologies under various conditions.

It is therefore necessary to integrate the modular analysis within a more comprehensive framework which allows assessment of the fundamental industry decisions with regard to utilization of modules. This comprehensive framework is displayed in Figure 2. The diagram is intended to show the major technical and economic areas and interrelationships which must be integrated. It demonstrates the key role, as a driving force, of policy analysis and scenario development (represented by the exogenously specified inputs to each model component). Potential demand for electricity and costs of alternative methods for meeting this demand under environmental and other constraints are shown to be the basis of utility decisions. These decisions determine the course of industry development and the consequences which may flow from this course, including effects on human populations and ecosystems as well as socioeconomic effects.

Figure 2 has been constructed in two sections. The section above the dotted line shows the configuration of components and information flows for simulation of the development and operation of an electric utility system. By proper definition of the system, it is possible (with some important limitations) to conduct simulations on a regional, multiregional or national basis. Inspection of the components in the upper part of Figure 2 reveals that only economic, technical and environmental policy decisions are involved. The simulation of physical, chemical and biological phenomena, which must be addressed on a site-specific basis, is described by the configuration of components below the dotted line. This method of display has been selected in order to demonstrate clearly how economics and policy affect decisions concerning the type, quantity and location of power production facilities and the manner in which they are operated. A realistic assessment of how future developments in the electric utility industry will affect environmental quality must include an estimate of industry response to alternative policies as well as simulation of the production, dispersion, transformation and effects of environmental pollutants.

The lower portion of Figure 2 shows the configuration of components and information flows for simulation of the release, transport and transformation of air pollutants and determination of populations exposed. The modeling effort must be carried out on a site-specific basis. Thus, the information developed by the system simulation in the upper

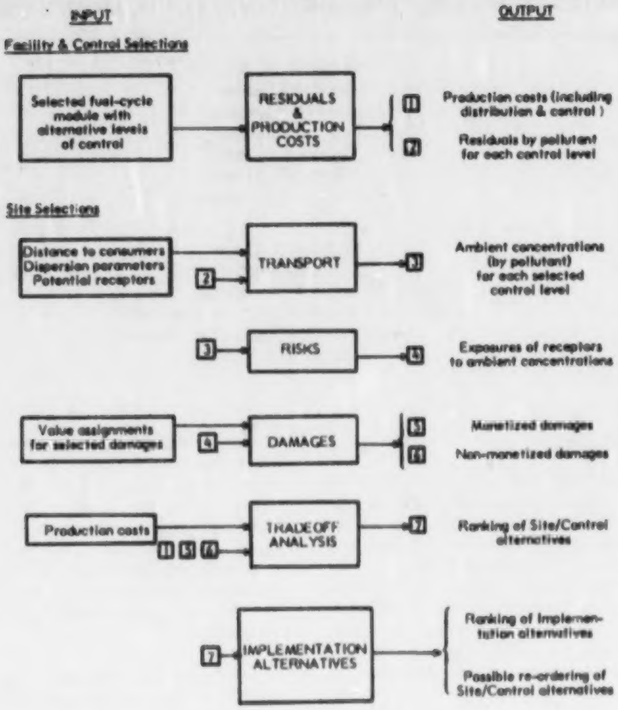
INPUT
OUTPUT
Facility & Control Selections
Selected fuel-cycle module with alternative levels of control
RESIDUALS & PRODUCTION COSTS
1
Production costs (including distribution & control)
2
Residuals by pollutant for each control level
Site Selections
Distance to consumers
Dispersion parameters
Potential receptors
2
TRANSPORT
3
Ambient concentrations (by pollutant) for each selected control level
3
RISKS
4
Exposures of receptors to ambient concentrations
Value assignments for selected damages
4
DAMAGES
5
Monetized damages
6
Non-monetized damages
Production costs
1
5
6
TRADEOFF ANALYSIS
7
Ranking of Site/Control alternatives
7
IMPLEMENTATION ALTERNATIVES
Ranking of Implementation alternatives
Possible re-ordering of Site/Control alternatives

Figure 1. Elements in Scenario Specification

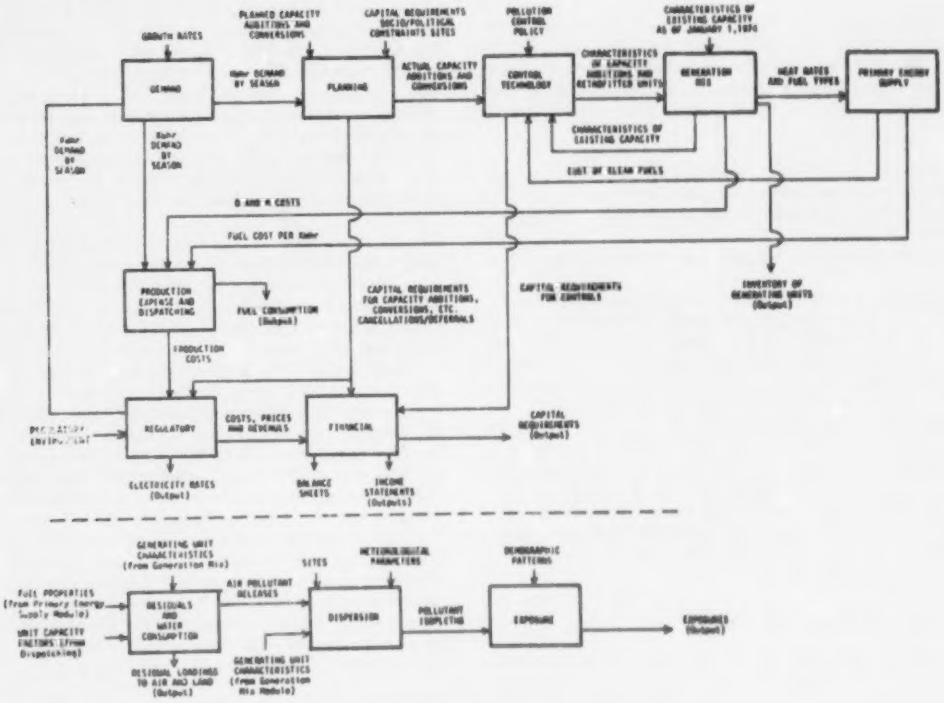
GROWTH RATES
DEMAND
KWhr DEMAND BY SEASON
PLANNED CAPACITY ADDITIONS AND CONVERSIONS
CAPITAL REQUIREMENTS SOCIO/POLITICAL CONSTRAINTS SITES
PLANNING
ACTUAL CAPACITY ADDITIONS AND CONVERSIONS
POLLUTION CONTROL POLICY
CONTROL TECHNOLOGY
CHARACTERISTICS OF CAPACITY ADDITIONS AND RETROFITTED UNITS
CHARACTERISTICS OF EXISTING CAPACITY AS OF JANUARY 1, 1976
GENERATION MIX
HEAT RATES AND FUEL TYPES
PRIMARY ENERGY SUPPLY
CHARACTERISTICS OF EXISTING CAPACITY
COST OF CLEAN FUELS
KWhr DEMAND BY SEASON
KWhr DEMAND BY SEASON
O AND M COSTS
FUEL COST PER KWhr
PRODUCTION EXPENSE AND DISPATCHING
FUEL CONSUMPTION (Output)
CAPITAL REQUIREMENTS FOR CAPACITY ADDITIONS, CONVERSIONS, ETC. CANCELLATIONS/DEFERRALS
CAPITAL REQUIREMENTS FOR CONTROLS
INVENTORY OF GENERATING UNITS (Output)
PRODUCTION COSTS
REGULATORY ENVIRONMENT
REGULATORY
COSTS, PRICES AND REVENUES
FINANCIAL
CAPITAL REQUIREMENTS (Output)
ELECTRICITY RATES (Output)
BALANCE SHEETS
INCOME STATEMENTS (Outputs)
GENERATING UNIT CHARACTERISTICS (From Generation Mix)
FUEL PROPERTIES (From Primary Energy Supply Module)
UNIT CAPACITY FACTORS (From Dispatching)
RESIDUALS AND WATER CONSUMPTION
AIR POLLUTANT RELEASES
SITES
METEOROLOGICAL PARAMETERS
DISPERSION
POLLUTANT LOADINGS
DEMOGRAPHIC PATTERNS
EXPOSURE
EXPOSURES (Output)
RESIDUAL LOADINGS TO AIR AND LAND (Output)
GENERATING UNIT CHARACTERISTICS (From Generation Mix Module)

Figure 2. Module Diagram and Information Flows in the ITA Model

portion of Figure 2 must be disaggregated so as to drive the site-specific models shown in the lower portion of the figure.

Scenario Development

The exogenously specified inputs to the components displayed in Figure 2 are elements of the various scenarios which are being addressed in the ITA.

By the term "scenario" we mean a specification of future events or conditions which is sufficiently complete to allow an evaluation of principal costs to the industry and consumers, effects on air quality, cost effectiveness of pollution control alternatives, and resource consumption that will occur if these events or conditions do, in fact, come about. Our focus is on the pollutants released and resulting human exposures. Releases depend on a number of diverse factors which may be grouped under the headings of economics, technology and policy.

For example, the chemical species and quantities of pollutants released depend on the fuels used, the design of generating units and the total amount of electricity produced. These, in turn, are dependent upon general economic conditions and the market prices for the fuels which compete for usage by utilities. Given production levels, generating unit characteristics and the properties of fuels, pollutant releases depend upon the technology employed for electricity production and the effectiveness of any control technology employed. Environmental policies such as mandated emission limits affect pollutants released from any one source. Energy policy affects production insofar as the price and availability of fuels are concerned. More direct effects on production may results from efforts toward conservation, electrification or load management.

Exposures also depend on when and where pollutants are released and on demographic patterns. Timing of releases depends on the temporal pattern of demand which may be affected by policies of demand management. Siting of sources is affected by economic, technological and policy constraints. Siting flexibility depends on the existence of cost-effective technology for long distance transmission. Environmental controls may take the form of siting restrictions.

Table I presents, in outline form, the principal elements to be considered in specifying a scenario. Elements to be considered are grouped under the four headings of Economics, Technology, Siting and Policy. Complete specification of a scenario requires hypothesizing specific occurrences under each of the headings.

For the first year's effort, an initial list of 25 scenarios has been prepared by postulating specific occurrences for the scenario elements identified in Table I. This list will be subject to further refinement as the modeling effort proceeds.

Figure 3 exhibits the 25 selected scenarios in event tree format. In selecting these scenarios, the first criterion was the elimination of the less probable combination of elements and the second was selection of those most clearly focused on the environmental problems associated with usage of coal. In the second and third years, greater emphasis will be placed on other scenarios.

The 25 scenarios displayed in the figure have been grouped in five sets for convenience in discussion. The lettered elements correspond to the list provided in Table I. The rationale for each group is as follows:

Group A. This group provides a basis for comparison of policies on a more or less "business as usual" basis. A high economic growth rate with responsiveness to utility needs in price setting is postulated with no major effective programs for conservation. These conditions have been typical of the last two decades, although not representative of the very recent past. A high degree of dependence on either nuclear power or coal for baseload additions is postulated with conversion of gas fired power plants to oil. The policy options of baseline and relaxed controls (P_1 and P_2) and maximum controls (P_4) with one intermediate level (P_3) provide a range with which to evaluate possible costs and benefits of alternate levels of control. These policy options are combined with two siting alternatives in order to reflect differences in the populations subjected to, or protected from, exposure to pollutants.

Group B. This group provides a contrast to Group A in terms of showing how air pollution may be reduced from the Group A baseline by factors other than control policies. A slow economy is predicted with emphasis on conservation together with a high degree of dependence of nuclear power.

Group C. This group provides a contrast to Group A with respect to costs. A slow economy, emphasis on conservation and nonresponsive regulatory policies are predicted. Extensive dependence on coal is assumed. Control options are imposed under these conditions of financial adversity for utilities.

Group D. Group D includes an electrification policy so that growth in electricity usage is greater than in Group A. This growth could result from the occurrence of several events such as deployment of electric automobiles, increased use of electric space conditioning and extensive curtailment of natural gas supplies. Extensive dependence on either nuclear or coal for baseload additions is investigated under conditions of natural gas curtailment (which would contribute to the need for electrification). The more stringent control policy, P_4, is used together with the baseline control level, rather than P_3, as being more consistent with the increase in pollutant releases that would be a result of the thrust toward electrification.

Group E. Group E provides a contrast to Group D by isolating the impact of the movement toward electrification. It posits continued effective emphasis on conservation with other elements the same as for Group D.

This listing of scenarios is subject to change throughout the ITA. Individual scenarios may be dropped and others added. The basic framework is expected to remain unchanged. Of course, all the elements require extensive analysis to develop the quantitative specifications.

Description Of Components In The Simulation Framework

Specification of scenario elements provides the driving force for the individual components in the simulation framework displayed in Figure 2. The role of each component and the inputs to and outputs from each component are described below.

Electricity Demand

Demand for electricity in future years is the fundamental determinant of utility growth. Demand is thus a determinant of all economic and social costs and benefits actually accruing under any control policy. Forecasts used in the ITA are being carefully evaluated. Forecasting alternatives include extrapolation of past trends (including factoring judgments of expert individuals or bodies), econometric predictions and technology forecasts.

The Demand Component specifies electricity demand by season for each year and region of interest. Demand by season is specified using a typical daily load shape curve for each season and region of interest.

Table 1. Elements in Scenario Specification

Economics	Technology	Siting	Policy
Group I: High growth rate, favorable conditions for utility financing and: e_1 - No significant effect on pattern or level of demand through policy initiatives. e_2 - Continuing and effective conservation efforts aimed at both pattern and level of demand. e_3 - Effective measures toward increased electrification. Group II: Low economic growth rate with emphasis on conservation and: e_4 - A regulatory policy responsive to needs to attract investment to the industry. e_5 - A regulatory policy of restrained and delayed price increases which translates into a curtailment of earnings.	t_1 - Extensive dependence on nuclear power for baseload additions. Natural gas plants convert to oil. t_2 - Extensive dependence on coal for baseload additions. Natural gas plants convert to oil.	s_1 - No change in the current balance of considerations regarding remote versus near load center siting. s_2 - An increase in remote siting due to technical breakthroughs or policy decisions.	p_1 - Baseline controls; air quality standards are attained by limiting emissions. p_2 - Relaxed controls; air quality standards are attained utilizing tall stacks and intermittant constrols. p_3 - More stringent controls on precursors of sulfates. p_4 - More stringent controls on all air pollutants.

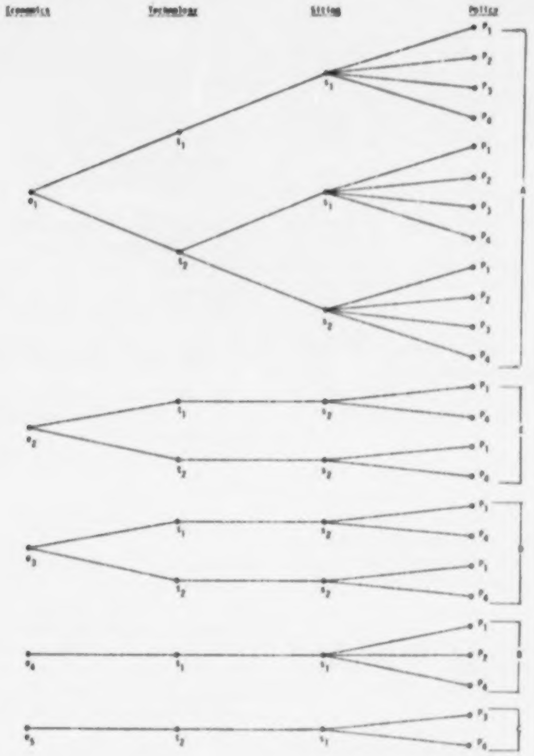

Figure 3. Scenarios for First Year ITA

Inputs—Growth rates in energy demand for each region, "regional" average load factor and load shape curves for each season.

Outputs—Energy and peak demand by region and season (to Planning, Production Expense, Dispatching and Regulatory Components).

Planning

Future capacity additions and conversions are being determined in accordance with announced plans of electric utilities and modified to reflect different postulated growth rates, capital requirements, and siting and sociopolitical constraints. Control policies as well as economic rationale are being considered both with regard to environmental protection and programs aimed at national energy self-sufficiency.

Inputs

- Demand (from Demand Component).
- Conversions, i.e., from oil to coal, from gas to coal, etc.; Planned Capacity Additions; Capital Costs; Socio/Political Constraints; Generating Unit Sites (exogenous inputs).

Outputs to Control Technology and Generation Mix Components:

- Planned conversions (oil to coal, gas to oil).
- New units by type brought on-line in a given year.

Outputs to Financial and Regulatory Components:

- Capital requirements for construction of units and control devices.
- Cancellation, deferral or acceleration of units scheduled to come on-line in future years.

Control technology

Alternative methods for air pollution control are being specified in terms of costs and capabilities. Modeling reflects both the consequences of pollutant shifts from one medium to another and the possibility for creation of new pollutants as a by-product of control.

The Control Technology Component specifies costs, efficiency and impact on plant operation of pollution control alternatives for SO_2, NO_x, particulates, and chemical and thermal effluents.

Inputs

- Capacity additions and conversions (from Planning Component).
- Characteristics of existing capacity (from Generation Mix Component).
- Degree of control required (exogenous input).
- Cost of clean fuels (from Primary Energy Supply Component).

Outputs

- Costs for meeting a given emission or effluent standard (to Financial Component).
- Characteristics of capacity additions and retrofitted units (to Generation Mix Component).
- Degree of pollution control (to Residuals Component).

Generation Mix

Most recently available characteristics of existing capacity are being specified on the basis of Federal Power Commission data as updated by information from utilities. Component input includes the characteristics of planned capacity additions and modifications to existing capacity to reflect fuel conversions and retrofits for pollution controls. The Generation Mix Component is essentially a file which contains the characteristics of generating units for any particular year of interest to the ITA.

The Generation Mix Component specifies the capacity profile as of 1974. It is updated during the simulation to show the "state of the system" for each year of interest in the future.

Inputs—characterization of existing capacity as of January 1, 1974 (data available from FPC) according to:

- Size
- Age
- Type and composition of fuel(s)
- Heat rate
- Type of air pollution controls
- Type of cooling
- Stack height
- Location
- Ownership
- Status of Section 316(a) application
- Capacity factor
- O & M expense
- Source of fuel

Inputs—data available from other sources:

- Characteristics of additions to generating capacity according to size, fuel type and composition, type of pollution control, etc. (from Planning Component).
- Retirements and re-rates (from Planning Component).

Outputs

- Inventory of generating units (output).
- Generating unit characteristics (to Residuals Component and Control Technology Component).
- Heat rates and fuel types for each class of facility (to Primary Energy Supply Component).
- O & M costs (to Production Expense and Dispatching Component).

Primary Energy Supply

The chemical and physical characteristics and delivered costs of primary fuels are being specified according to source of supply. This facilitates the identification and assessment of environmental and socioeconomic impacts associated with fuel extraction and processing to be conducted in years two and three of the ITA.

The Primary Energy Supply Component specifies the cost of available fuels for each generating unit.

Inputs

- Heat rates and fuel types for each facility (from Generation Mix Component).

Outputs

- Fuel cost per kilowatt hour generated for each facility (to Production Expense and Dispatching Component).
- Cost of clean fuels (to Control Technology Component).

Production Expense and Dispatching

Generating units are not operated in isolation; they function as part of an integrated system in which production is allocated to units to meet demand which varies by time of day and by season. Introduction of pollution controls which affect efficiency will cause shifts of load among units. In coming years, there may be attempts to change load curve shapes through special pricing regulations. Changes in allocation of load (e.g., between peaking and base load units) may radically change pollutant characteristics. Seasonal production patterns, of course, fundamentally affect the release of pollutants and, consequently, exposures. The dispatching of load plus the operating characteristics of a generating unit determine the expense incurred by the utility and, thus, the costs borne by the consumer. The ITA utilizes a simple dispatching model to determine capacity factors and production expenses.

The Production Expense and Dispatching Component calculates generating costs for each class of unit and specifies capacity factors such that the demand is met at least cost.

Inputs

- Fuel cost for each class of unit (from Primary Energy Supply Component).
- O & M costs for each class of unit (from Generation Mix Component).
- Demand by season (from Demand Component).

Outputs

- Fuel consumption for each class of unit (output).
- Capacity factors for each class of unit (to Residuals Component).
- Production expenses (to Regulatory Component).

Regulatory

The effects of regulatory policies on the financial and operating characteristics of utilities are being considered. This includes consideration of alternative pricing schemes and regulatory lag. The methods of treating production cost pass-through and financing of construction work-in-progress will affect the rate of utility response to needs for pollution controls, capacity additions and fuel conversions.

The Regulatory Component specifies electricity rates consistent with recovery of production costs and a return on rate base.

Inputs

- Production expenses (from Production Expense and Dispatching Component).
- Demand for electricity (from Demand Component).
- Regulatory environment (exogenous input).
- Rate base and financial needs (from Financial Component).

Outputs

- Electricity rates (output).
- Production costs, prices and revenues (to Financial Component).

Financial

Costs of both new facilities and of pollution control equipment are being evaluated in the context of utility financing. Needs for capital, ability to finance capital expansion, earnings and the ability to recover capital and operating costs in revenues are basic considerations in industry decisions with regard to development. The impact of control policies is being measured in terms of effects on needs for capital, earnings, prices and return on investment. The fundamentally different financial structures of investor owned and non-investor owned utilities require that simulation of the financial impacts of future environmental policies treat the two types of firms separately.

The Financial Component calculates financial flows and updates balance sheets and income statements each year.

Inputs

- Initial balance sheet (exogenous input).
- Profit and loss items (exogenous input).
- Rate schedules (from Regulatory Component).
- Production costs and revenues (from Regulatory Component).
- Capital requirements (from Planning Component) for new capacity, transmission, distribution and plant conversions.
- Capital requirements for pollution control equipment (from Control Technology Component).

Outputs

- Updated balance sheets and income statements for each year (output).
- Aggregate capital requirements (output).

Residuals And Water Consumption

Existing data bases for the residual releases from power plant operation are being refined and assigned to existing and new facilities. Generating unit characteristics and fuel properties are being considered in order to define residual release rates as functions of these independent variables. The residuals model not only considers the removal efficiencies of control equipment, but also reflects increased residual releases due to reduction in plant efficiency resulting from control technology application. The first year's effort focuses on air pollutants, especially SO_2, NO_x, and primary particulates. Other residuals considered will include trace elements and waste heat. Cross-media effects are also considered.

Since calculation of evaporative water consumption requires some of the same inputs as residuals generation, it is included in this component.

Inputs

- Unit capacity factors (from Production Expense and Dispatching Component).
- Properties of the fuels (from Primary Energy Supply Component).
- Characteristics of the generating unit (from Generation Mix Component).
- Characteristics of control devices (from Generation Mix Component).

Outputs

- Air pollutant release rates from each generating unit (to Dispersion Component and output).
- Water consumption rate for condenser cooling (output).
- Solid waste generation rates (output).
- Waste heat discharged (output).

Dispersion

Pollutants are being traced from release at the power plant to eventual impact on sensitive receptors. Chemical transformations and interaction with other materials in the environment will be included in the assessment. The first year's study considers the dispersion of air pollutants only. In view of the results of very recent research, a major emphasis must be placed on transport of pollutants on an inter-regional scale (i.e., 100 to 1000 miles from the source).

The Dispersion Component calculates changes in local air quality due to releases of pollutants calculated in the Residuals Component. Separate models are provided for short range and long range atmospheric transport.

Inputs

- Release rates for each air pollutant (from Residuals Component).
- Stack parameters for each generating unit (from Generation Mix Component).
- Location of each generating unit (from Generation Mix Component).
- Local meteorological parameters (exogenous input).

Outputs

- Ambient concentrations of air pollutants at distances less than 50 km from the generating unit. Concentrations are specified according to location parameters, e.g., census tract, zip code, county (to Exposure Component and output).
- Contributions to sulfate concentrations in selected impact areas greater than 100 miles downwind from the generating units (to Exposure Component and output).

Exposure

Populations at risk to air pollutants for specific geographical regions are being identified such that projected patterns of demographic growth correspond to growth in regional demand for electricity. The demographic modeling reflects changes in national fertility rates as well as secular economic trends. Since populations at risk are defined in terms of the spatial relationship between sources and receptors and the conditions of pollutant transport, the interaction of siting, residuals and air dispersion models is crucial to exposure model development.

The Exposure Component calculates populations exposed to increments in ambient pollutant concentrations.

Inputs

- Pollutant isopleths (from Dispersion Component) according to locational parameter (census tract, zip code, etc.).

Outputs

- Populations exposed to specified levels of pollutant concentrations.

ENVIRONMENT IMPACT MODELLING FOR PROJECT INDEPENDENCE

R. A. Livingston
Office of Planning and Evaluation
U. S. Environmental Protection Agency
Washington, D.C.

G. R. Kendall
Teknekron, Inc.
Berkeley, California

R. W. Menchen
Hittman Associates, Inc.
Columbia, Maryland

H. P. Santiago
Office of Planning and Analysis
Federal Energy Administration
Washington, D.C.

I. SUMMARY

An application of the environmental residuals technique for evaluating the environmental implication of energy policy studies is described. This paper covers the adaptation of the techniques to the particular needs of the Project Independence Evaluation Systems, some typical results of the analysis, and its limitations. Several different methods of scenario and residual comparison are investigated. The conclusions are that the residuals approach can be a useful tool in comparing alternative scenarios, but a tradeoff must be made between degree of detail and comprehension of results. Areas for further work include extension of residuals to cover more items of interest, introduction of time dependency, and development of aggregate measures for comparison.

II. BACKGROUND

This project arose from Environmental Protection Agency's participation in the Project Independence interagency effort initiated in March of 1974 to evaluate national energy problems and provide a framework for developing a national energy policy. The effort assembled a comprehensive energy data base, developed a methodology for analyzing future energy supply and demand alternatives, and investigated the impacts and implications of major energy strategies.[1]

The results of the initial study were presented to the President in December 1974. Subsequent studies utilizing the Project Independence Evaluation System (PIES) were published in connection with the Draft Environmental Impact Statement for the Energy Independence Act, March 1975,[2] and the current version of the Project Independence Report.[3]

EPA was given the responsibility of assessing the environmental impacts of the energy scenarios produced by PIES. The assessment had to be performed rapidly, repetitively and in a consistent fashion. The assessment of the scenario had to be done using quantitative techniques as much as possible.

III. CONSTRAINTS ON ANALYSIS

A. PIES Model and Scenario Constraints

The Project Independence Evaluation System (PIES) is a set of computer models of the technologies, demand and the markets through which energy commodities are extracted, transported, transformed and consumed. Regional production, processing and conversion activities are represented within the energy network as nodes, with links depicting transportation and distribution possibilities. The PIES model simulates a market system which takes into account prices, resource requirements and capacity constraints, and constricts a set of energy flows that satisfies the final demands for energy. It is a least cost linear program. PIES models energy supply side and adjusts prices (thus demands) until the system achieves an equilibrium balance at which no consuming sector would be willing to pay more for an additional unit of any energy product, and no supplies would provide an additional unit of any energy product for less than the prevailing prices.[4]

An individual energy scenario is developed on the PIES model by inputting a set of supply and demand data representing particular energy policies or conditions, including the world price of oil. The system then computes a least cost solution and provides the output in terms of quantities produced and consumed, with associated prices. The solution applies only to one point in time and for one world price of oil. The PIES system is not a dynamic model.

B. PIES Output Constraints

The PIES output becomes the data base for the environmental assessment. However, it was designed to suit the objectives and data availability of the energy analysis, and these did not necessarily correspond to the needs of the environmental analysis. The information content and structure of the PIES output thus constrained the scope of the subsequent environmental information.

On the supply side, the PIES output gave production statistics on an individual region basis for coal, oil, natural gas, and U235 extraction. However, the regions for each energy source were based upon traditional boundaries, as defined by the relevant source of statistics. For example, coal was organized by the Bureau of Mines coal provinces, petroleum and natural gas by NPC petroleum provinces and so on. Similarly, oil refining was broken down by Petroleum Administration Districts (PAD) and electricity by Electric Reliability Council regions. Generally, the regional boundaries of one activity did not coincide with that of another, which prevented a direct comparison of energy scenarios on a geographical basis.

Second, the PIES output specified only the total quantity of activity for a particular region, without specifying the size of the facilities or their geographic location within the region. For example, oil refining activity was described as total barrels of throughput in a PAD. This production could be distributed in any number of locations from Delaware to Florida, and in any size facility from 10,000 to greater than 250,000 barrels per day.

Finally, source factors significant from an environmental viewpoint, such as sulphur content of coal, were not given in the output.

C. Environmental Data Constraints

In addition to the limitations imposed on the environmental analysis by the PIES output, the analysis was further constrained by the availability of quantitative environmental data, and methodological problems of environmental analysis. Warner and Preston in their 1974 review of environmental impact assessment methodologies, identified 17 different approaches to environmental impact assessment and concluded that there was "no universally applicable procedures for conducting an adequate analysis."[5]

Similarly, a number of studies have attempted to compile the environmental data related to energy on a systematic basis.[6,7,8,9] They differed among each other in sources of data, assumptions, pollutants covered and method of aggregation.[10] For the purposes of the Project Independence analysis, it was decided to use the data base prepared by Hittman Associates for the Council on Environmental Quality. It was felt that this provided the most thorough, flexible and widely utilized set of data available at the time. However, in making this choice, the environmental analysis was then limited to the set of pollutants as specified in the CEQ study. This covered seven water pollutants, and six air pollutants, as well as land use, solid waste, and occupational health.

D. Constraints of Project Independence Organization

The scope of the environmental analysis was also limited to a certain extent by the role of EPA's task force within the overall structure of Project Independence. In total there were 21 interagency task forces set up to address various aspects of energy supply and demand. In particular, questions related to water use and availability were assigned to the Water Resources Council and some socio-economic matters were assigned to a Manpower Task Force headed by the Labor Department.[11]

The other aspect of the Project Independence organization that limited the scope of the environmental analysis was the schedule, which originally allotted two months for the entire process of development and analysis of energy scenarios. This ruled out the development of any major new environmental techniques, and required that the environmental analysis involved be capable of being done in a short time.

IV. OBJECTIVE OF ENVIRONMENTAL ANALYSIS

Given the constraints outlined above, several objectives were chosen as a basis for designing a methodology for doing the environmental evaluation. These were:

A. Emphasis on Interscenario Comparison

The primary purpose of the environmental evaluation was to enable energy policy makers to appreciate the relative environmental ranking of different strategies to solve energy problems. However, this does not require that absolute environmental quality be predicted for a given scenario.

B. Level of Analytical Detail Consistent with PIES Output

The PIES Model operated on an aggregated regional basis, and looked at macroeconomic questions. The general lack of site specific information for energy production or consumption ruled out dispersion modelling or health effects calculation for measuring environmental impact. To do so would have produced spurious accuracy, not supported by the quality of information available.

C. No Environmental Constraints in PIES Model

A theoretically rigorous energy model should take into account the effect of environmental regulations and limitations on energy supply and consumption. However, this was not an objective for the Project Independence evaluation for two reasons. The first was the problem described of accurately calculating environmental quality with the data available. The second was the economic basis of the PIES model. Entering environmental variables into the model's calculation would have required coverting environmental impacts into external social costs. While theoretical models exist for calculating external costs,[12] a satisfactory practical method was not available.

D. No Preemption of Environmental Impact Statement

The environmental analysis performed in this project was not intended to satisfy the requirements of the EIS. This was partly because the Project Independence effort was a policy study, not involving specific physical activities which could be identified as requiring an EIS. Another reason was to avoid the possibility that by doing an EIS for Project Independence as a whole, individual projects could be relieved of the responsibility of having to do specific EIS.

E. Rapid Response

Since the environmental evaluation came at the end of the process of generating energy scenarios, it would inevitably have a very short timeframe for analysis before the final report would be written. Therefore, it became essential to be able to do the evaluation on short notice, in a rapid fashion.

V. ANALYTICAL APPROACH

Given the constraints and objectives outlined above, the environmental evaluation evolved into a comparison of energy scenarios using discrete residuals on a consistent regional basis.

A. Residuals

The term "residuals" means any measurable quantity which is associated with a given activity, and which results in environmental impacts. Air pollutants and water pollutants are included in this definition, as well as things such as land use, solid waste, water use, and manpower, which are not usually considered pollutants. Unquantifiable items like esthetics are not considered to be residuals.

It should also be noted that residuals are the precursors of environmental impacts and not the impacts themselves. For instance, the SO_2 emitted by a power plant is a residual, but the health effects caused by that SO_2 are an environmental impact. The number of acres of land disrupted by strip mining is a residual, but the loss of the ecosystem on that land is an environmental impact, and so on. Thus, the definition of residuals avoids the problems and uncertainties of calculating transport of pollutants and their effects.

Finally, by eliminating any reference to local environmental conditions, such as terrain, meteorology , population, etc. it becomes possible to conceptualize and compare representative energy activities rather than being forced to speak in terms of a particular coal mine or a particular power plant. This aspect is important when analyzing future energy choices, when the exact location of an activity is unknown, thus making it impossible to calculate the changes in ambient environmental conditions such as air quality or water quality. However, it is possible to compare the residuals associated with the alternatives since these are independent of location.

Thus, the advantages of residuals are that they deal in measurable, predictable quantities, in an objective way. Subjective elements, such as the ultimate environmental impact, or the relative weighting of different pollutants, are not considered. However, if one wishes to proceed to this kind of analysis, it is still necessary to know the residuals as the first step.

Furthermore, this makes it possible to trace back through all the steps involved in producing and transporting, converting, and consuming energy. Thus residuals analysis can account for all the associated pollution that may not occur at the power plant or other energy facility, itself, but that must also be charged to the production and consumption of a unit of energy.

In practice, the residuals technique involves a matrix of coefficients. One dimension of the matrix is energy activities, the other the residuals of interest. Each element in the matrix thus relates the production of a given residual to the throughput of energy involved in a specific activity. Separate matrices are developed for each major energy type. A sample coefficient matrix for coal is presented in Figure 1. It is necessary to define a vector, E_i, composed of a set of variables e_{ij} which describes a quantity of energy in a specific series of steps, or trajectory, from mining or extraction, to end use. The subscripts thus describe the jth step, eg. mining, in the ith energy source eg. coal. Then by multiplication, the total set of residuals, r_{ik} associated with this trajectory can be calculated:

$$(1) \qquad r_{ik} = e_{ij} \cdot m_{ijk}$$

However, since more than one energy trajectory is usually involved, each with its characteristic residuals matrix, the total residuals for an energy scenario are:

$$(2) \qquad r_{ik} = \sum_j \sum_i e_{ij} \cdot m_{ijk}$$

However, equation (2) should be modified in the case of Project Independence analysis to take into account the regional nature of the energy reserves. Thus for region 1, the residuals are:

$$(3) \qquad r_{kl} = \sum_j \sum_i e_{ijl} \cdot m_{ijkl}$$

Since each type of energy production specified in the PIES output had its own set of regions, it was also necessary to introduce an allocation factor a_{iql} such that:

$$(4) \qquad r_{kl} = a_{iql} \sum_j \sum_i e_{ijq} \cdot m_{ijlq}$$

Thus in order to arrive at a quantitative measure of the residuals associated with a given energy a set of regionalized , energy specific residual matrices had to be generated as well as a set of allocation factors to convert from energy regions into a consistent set of regions for residuals analysis. The residuals matrices were developed under contract by Hittman Associates, Inc., utilizing residuals matrices developed under a previous contract for CEQ[13], and modified to suit the specification of PIES. This effort is described in a separate paper.[14]

B. Regional Allocation System

From equation (4) it can be seen that the set of uniform regions into which the various energy regions are allocated, must be a common subset of each energy region. These uniform regions must also make sense from an environmental standpoint. This task was assigned to another contractor ERCO (Energy Resources Co.).

The basic question to be decided was which type of region should be used. Air Quality Control Regions (AQCR) were not used originally because their boundaries were drawn along political subdivisions rather than topographically separate regions, and because in some cases, they covered too broad an area. Instead it was decided to use river basins, as defined by the National Oceanographic and Atmospheric Administration. These basins represented national regions for water quality analysis, and their physical boundaries also provided a fairly good basis for air sheds.

The development of the river basins model and the allocation procedure is described in more detail in a separate paper.[15] Subsequently, a subroutine was added to the model which provides the ability to allocate the residuals to AQCRs.

C. Other Considerations of Residuals Analysis

1. Energy End Use--In the initial Project Independence effort, the environmental evaluation associated with the end use of energy was not considered, although impacts associated with electrical generation were included. End uses were not considered primarily because the Project Independence effort concentrated on supply options to meet a given level of demand. Thus the level of demand was essentially not within the control of policy measures under consideration. The environmental evaluation was intended to bring home the effect of conscious decisions on the part of policy makers. Secondly, the amount of effort required to produce end use residuals matrices and allocation models was not available in this phase of the project. However, in subsequent efforts, the end use environmental evaluation was implemented and used.

2. Nuclear Energy--A set of residual coefficients were derived to describe the non-radiological aspects of nuclear energy, primarily U-235 extraction and operational releases of radioactivity from power plants. No overall analysis of radioactivity was made. This was because of the difficulties of comparing the production and decay over time of radioactivity with other residuals. Also, the level of nuclear power usage was relatively constant among energy scenarios, and thus would have little effect on their relative ranking.

3. Environmental Control Standards--It was assumed that all environmental control regulations and standards promulgated up to the time of the Project Independence study could be in full effect in 1985, the point of time chosen for the analysis. This had the effect of reducing some water pollutants to zero, and minimized land use impacts from strip mining.

4. Socio-Economic Factors--No evaluation of the usual socio-economic factors was made, nor were analysis of environmental impacts of secondary development considered. This was done both because it was not within the scope of the environmental task force's responsibility and because it involved data which was not readily available.

D. Scenario Comparison

Once the residuals had been calculated and compiled on a consistent regional basis, it was necessary to find a technique to compare scenarios. A number of different techniques were considered.

1. Single Index-- The use of a measure which would aggregate all the individual residuals into a single index was considered and rejected. Although it would have provided a simple means of ranking the scenarios, it would have involved the use of weighting factors to be applied to the residuals. The state of the art has not advanced to the point where objective weighting factors are available, and judgemental ones would have introduced a subjective factor into the analysis. Moreover, it was felt that as much information as possible should be presented concerning the environmental impacts, and thus it was better to display the entire list of residuals, rather than a single number.

2. Overlays--An attempt was made to display the residuals as overlays on a national map. However, it proved impossible to present more than two pollutants at a time, or, alternatively, to compare more than two scenarios at a time (Figure 2). Moreover, the river basins introduced too much detail.

3. Tabular Presentation--The most successful approach on a regional basis was in the form of tables of residuals. In order to make the data manageable, the data from the river basins were aggregated into 14 major regions, corresponding to the demand regions used by FEA. An example of this format is presented in Figure 3. Here the method of comparison is simly to match the products to a particular residual from one scenario to another.

4. Graphical--The regional tabular method is the most straightforward. However, it tends to take up a lot of space and major trends are difficult to extract from the details. Consequently, in its publication on Project Independence, FEA resorted to presenting the residuals on a national basis in the form of bar charts. This is illustrated in Figure 4. While definitely simplifying the presentation and making it more comprehensible, this has the effect of discarding the information on regional impacts, which is one of the major objectives of the PIES approach.

5. Differential Comparison--As a way of overcoming some of the difficulties of the regional tabular approach, a matrix was prepared showing the differentials in residuals between two selected scenarios, one dimension are the individual residuals The matrix is presented in Figure 5. While it does provide a concise detailed comparison, its disadvantage is that it cannot be simply extended to comparison of three or more alternatives.

VI. RESULTS

It is not the intent of this paper to cover in a comprehensive fashion the results of the various scenario analyses, these can be found in the reports published by FEA,[16] and ERCO[17,18] and Hittman. However, there were some findings that kept recurring.

One is that on a national basis energy related pollutant loadings will either decline or remain constant between 1972 and 1985. This indicates the effect of meeting pollution control standards, and emphasizes the importance of accurate assumptions concerning the efficiency and degree of use of controls.

A second find, on a national basis, is that residual loadings variations among scenarios in 1985, tends to be less than the change between 1972 and 1985. From a national policy viewpoint, this suggests that the most useful effort should be on making sure that environmental standards are met, rather than attempting fine tune energy supplies to determine the most environmentally acceptable scenario.

Third, for some residuals, such as particulates, the loadings associated with different supply scenarios, are small in comparison with the quantities from end use activities. This suggests that more thought should be given to controlling end use emissions, and to energy conservation.

Fourth, some scenarios involving accelerated development had the effect of reducing some residuals over the business-as-usual scenarios in 1985. This apparently results from the more rapid retirement of older facilities with less stringent pollution controls, as well as switching away from coal to oil.

Finally, individual regions may show widely different environmental impacts within a given scenario and between scenarios. This indicates that comparing residuals solely on a national basis is not sufficient for evaluating environmental impacts.

VII. CONCLUSIONS AND RECOMMENDATIONS

The primary conclusion is that residuals analysis can be useful as a practical tool in comparing environmental impacts of energy alternatives. While it is not a substitute for a thorough study of particular regional or local impacts associated with a definite activity, it does provide quick "broad-brush" answers more in keeping with the generalized information produced in policy studies like Project Independence. It can be used as a way of identifying problem regions which should receive more indepth analysis. Care must be taken however to use residuals on a comparative rather than absolute basis.

There appears to be a definite tradeoff between the amount of detail involved in the analysis and the comprehensibility of the results. Although the environmental evaluation actually produces information for over three hundred subregions of the U.S., it becomes extremely difficult to relate this to the overall implications of energy policy. Consequently, a more aggregated comparison technique, at 10 subregions of the U.S. had to be carried out. Even then, it proved difficult to comprehend, and for the FEA reports, it proved necessary to resort to national summaries.

Areas for further work include developing a better methodology for comparing and presenting residuals and scenarios, so that the full capacity of the techniques can be utilized. Additional residual coefficients need to be developed for items like trace metals. Some more extensive emissions and monitoring data is needed before a simple and practical technique for converting residuals information into air and water quality results can be developed. Finally, the residual coefficients should be modified to reflect problems that are not at steady state with energy throughputs. These would include efforts that are cumulative over time, such as acid mine drainage, land use or radioactive wastes, or that are site sensitive, such as impacts due to construction.

Improvements in residuals modelling also implies improvements in energy modelling. This includes better regional descriptions, better characterization of industrial energy facilities, additional energy resource characteristics, and introduction of dynamic elements into the model.

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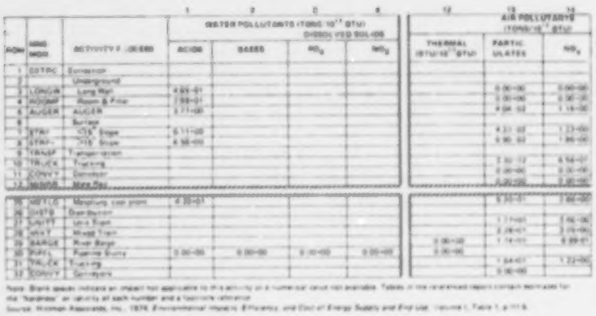


ROW	ABBR	ACTIVITY	WATER POLLUTANTS (TONS/10¹² BTU) 1 ACIDS	2 BASES	DISSOLVED SOLIDS 3 PO_4	4 NO_3	12 THERMAL (BTU/10¹² BTU)	AIR POLLUTANTS (TONS/10¹² BTU) 13 PARTICULATES	14 NO_x
1	EXTRC	Extraction							
2		Underground							
3	LONGW	Long Wall	4.85-01					[illegible]	[illegible]
4	ROOMP	Room & Pillar	7.98-01					[illegible]	[illegible]
5	AUGER	AUGER	3.77+00					[illegible]	[illegible]
6		Surface							
7	STRI	<15° Slope	6.11+00					[illegible]	[illegible]
8	STRP-	>15° Slope	6.56+00					[illegible]	[illegible]
9	TRNSP	Transportation							
10	TRUCK	Trucking						[illegible]	[illegible]
11	CONVY	Conveyor						[illegible]	[illegible]
12	[illegible]	Mine Rail						[illegible]	[illegible]
25	METLG	Metallurgical coal plant	4.20-01					[illegible]	[illegible]
26	DISTB	Distribution							
27	UNITT	Unit Train						[illegible]	[illegible]
28	MIXT	Mixed Train						[illegible]	[illegible]
29	BARGE	River Barge					[illegible]	[illegible]	[illegible]
30	PIPEL	Pipeline Slurry	0.00+00	0.00+00	0.00+00	0.00+00	[illegible]		
31	TRUCK	Trucking						[illegible]	[illegible]
32	CONVY	Conveyors						[illegible]	

Note: Blank spaces indicate an impact not applicable to this activity or a numerical value not available. Tables in the referenced report contain estimates for the "hardness" or validity of each number and a footnote reference.

Source: Hittman Associates, Inc., 1974. Environmental Impacts, Efficiency, and Cost of Energy Supply and End Use, Volume I, Table 1, p. II-5.

FIGURE 1. EXAMPLE OF RESIDUALS MATRIX FOR COAL MINING

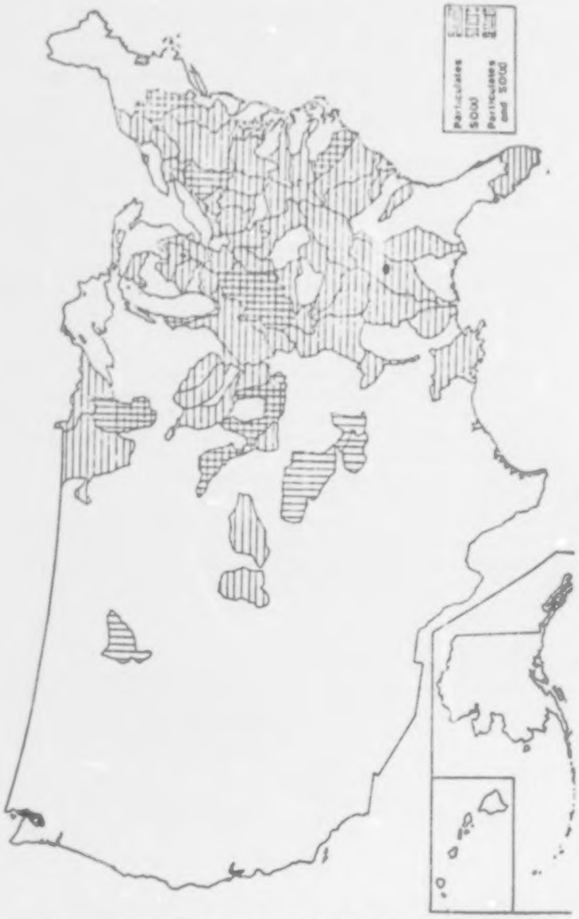
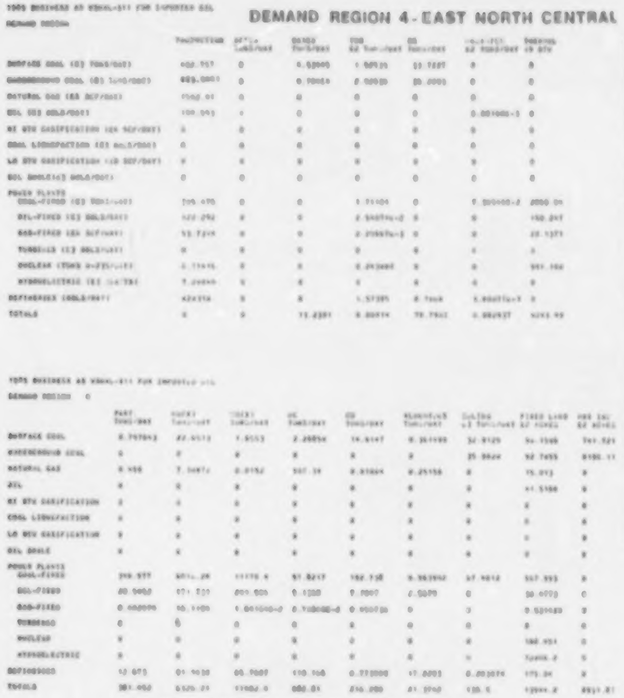
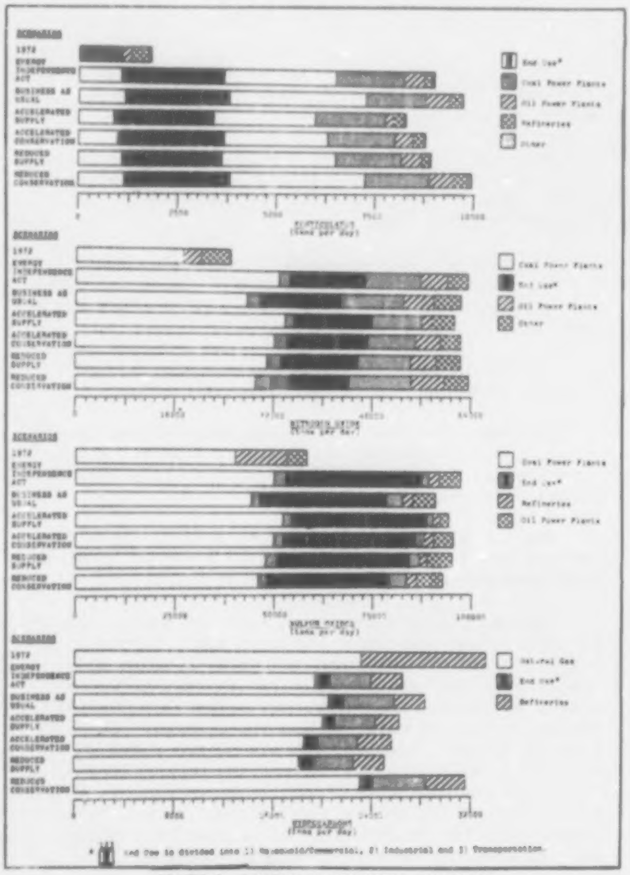


FIGURE 2. ACCELERATED SUPPL. SO_x AND PARTICULATES REGIONS EXCEEDING PRIMARY STANDARDS IN 1972 AND INCREASED LOADINGS IN 1985



DEMAND REGION 4 - EAST NORTH CENTRAL

FIGURE 3. EXAMPLE OF REGIONAL TABULAR COMPARISON



* End Use is divided into 1) Household/Commercial, 2) Industrial and 3) Transportation.

FIGURE 4. EXAMPLE OF GRAPHICAL COMPARISON

COMPARISON OF #11 SCENARIOS

	DEMAND REGIONS											TOTAL NO. (less Nat.)		
POLLUTANT	1	2	3	4	5	6	7	8	9	10	Nat.	A	B	-
Acids	-	-	-	-	-	-	-	-	-	-	-	0	0	10
Bases	-	-	A	A	A	-	-	-	-	-	A	3	0	7
TDS	-	-	A	A	-	-	B	A	B	-	A	3	2	5
SS	-	-	A	A	A	-	B	-	-	-	A	3	1	6
Organics	B	-	B	-	-	-	B	-	B	B	B	0	5	5
Thermal	-	-	-	-	A	-	-	-	-	-	-	1	0	9
Part.	-	-	A	-	A	-	-	-	-	-	-	2	0	8
NO_x	-	A	A	A	A	-	-	-	-	-	A	4	0	6
SO_x	-	-	A	A	A	-	A	-	-	-	A	4	0	6
HC	-	-	A	-	-	-	B	-	B	-	B	1	2	7
CO	A	A	A	A	A	-	A	-	-	-	A	6	0	4
Ald.	-	-	A	A	-	-	B	A	B	-	-	3	2	5
Solids	A	A	A	-	A	-	-	B	-	-	B	4	1	5
F-Land	-	-	-	-	-	-	-	-	-	-	-	0	0	10
I-Land	-	-	A	A	A	A	A	-	-	-	A	5	0	5
TOTAL NO.														
A	2	3	11	8	9	1	3	2	0	0	7	39		
B	1	0	1	0	0	0	5	1	4	1	3		13	
-	12	12	3	7	6	14	7	12	11	14	5			98

A = Accelerated Supply has less loading

B = Business as Usual has less loading

- = if difference between strategies is less than 5% or if difference between strategies is less than 1% of the National total of that pollutant in Business as Usual

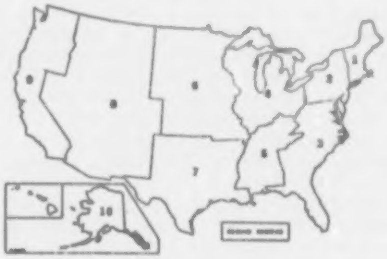


FIGURE 5. EXAMPLE OF DIFFERENTIAL COMPARISON

AN ENVIRONMENTAL RESIDUAL ALLOCATION MODEL

M. Allen F. Lambie
Energy Resources Co. Inc.
Cambridge, Massachusetts

Summary

An environmental residuals technique was developed to quantitatively evaluate the environmental implications of Project Independence. Three models are discussed that compare the regional impacts of different scenarios of energy development: a Residual Allocation Model to predict the quantity and distribution of 15 energy-associated pollutant loadings, a Water Use Model to assess the compatibility of water available and water required for projected energy use, and an Air Quality Model to compare the impacts of the scenarios on ambient air quality. The approach is useful for scenario comparison, but is limited in degree of detail and absolute accuracy. It is concluded that the level of control technology achieved is more critical environmentally than the choice of scenarios. Further work should include a refinement and extension of the residuals studied and a more detailed sensitivity analysis, especially with respect to control technology and facility siting assumptions.

Introduction

The viability of any long-range planning for national energy development rests in part on the critical nature of the environmental component. Although national strategies for developing energy resources must be chosen ultimately from the set of alternatives that are economically and technically practicable, the pressing nature of environmental problems dictates that, among such alternatives, the optimal choice should consider the relative environmental impacts of the strategies. Precisely this reasoning led to the formulation of a model by which to compare the environmental implications of the various scenarios generated by the Federal Energy Administration's (FEA) Project Independence Evaluation System (PIES) model[1,2,3]. This Residual Allocation Model, developed by Energy Resources co., assesses energy scenarios on the basis of the allocated levels and geographic distribution of pollution loadings associated with energy supply and the resulting end use patterns. In addition, a Water Use Model indicates for each scenario the general compatibility of energy-associated water demands with regional projections of water supply. Finally, an Air Quality Model evaluates emissions predicted by the Residual Allocation Model in terms of their impact on regional ambient air quality. (See Figure 1.)

The purpose of these models is to allocate predicted pollution loadings into common geographic areas so that the relative impacts of these loadings can be analyzed. The study considers 15 impact categories, or residuals, defined by the Environmental Protection Agency (EPA):

Air Pollutants
- Particulates
- Nitrogen Oxides
- Sulfur Oxides
- Hydrocarbons
- Carbon Monoxide
- Aldehydes

Water Pollutants
- Acids
- Bases
- Total Dissolved Solids
- Suspended Solids
- Organics
- Thermal Discharge

Land Use Parameters
- Solid Wastes
- Fixed Land
- Maximum Incremental Land

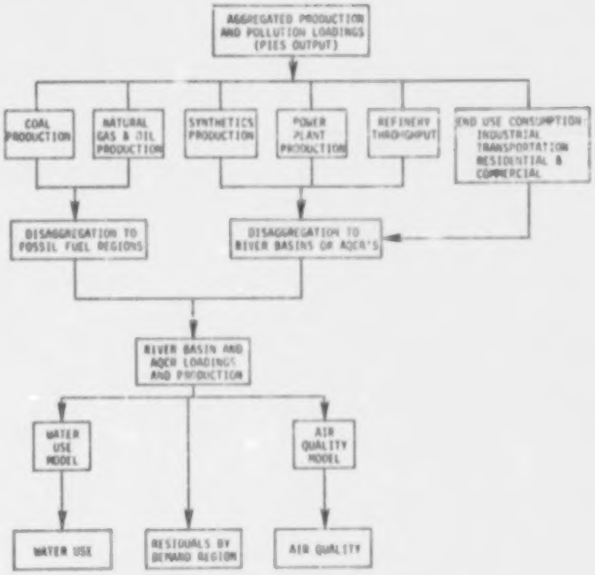

AGGREGATED PRODUCTION AND POLLUTION LOADINGS (PIES OUTPUT)
COAL PRODUCTION
NATURAL GAS & OIL PRODUCTION
SYNTHETICS PRODUCTION
POWER PLANT PRODUCTION
REFINERY THROUGHPUT
END USE CONSUMPTION: INDUSTRIAL TRANSPORTATION RESIDENTIAL & COMMERCIAL
DISAGGREGATION TO FOSSIL FUEL REGIONS
DISAGGREGATION TO RIVER BASINS OR AQCR'S
RIVER BASIN AND AQCR LOADINGS AND PRODUCTION
WATER USE MODEL
AIR QUALITY MODEL
WATER USE
RESIDUALS BY DEMAND REGION
AIR QUALITY

Figure 1 FLOW CHART FOR ENVIRONMENTAL ASSESSMENT

Projected regional levels of these residuals serve as the basic indicators of environmental quality. The analysis consists of five distinct stages:

1. The PIES Model predicts levels of energy activities and resulting pollution loadings for a given scenario. Unfortunately, the geographic regions used for each activity are different.

2. The Residual Allocation Model allocates these production and consumption levels and the associated pollution loadings among a consistent set of smaller regions.

3. Impacts of pollution loadings are analyzed at various levels of geographic aggregation.

4. The Water Use Model estimates regional energy-related water demand on the basis of scenario production levels; this demand is compared to projected regional water supply.

5. The Air Quality Model assesses scenario-related ambient air quality on the basis of regional loadings predicted by the Residual Allocation Model.

The models were developed with the particular aim of aiding time-constrained EPA and FEA analysts in the comparison of the environmental impacts of various scenarios. The need to guarantee realistic output useful to decision-makers required feedback between the conceptual formulation and the feasible approaches. Thus, a "paper" model was conceived, the required supporting data were sought, and the model was revised to accept the best data found to be available. As with most working models, the critical factor in this process was the availability of meaningful, reliable data at level of detail sufficient to support the allocation. Since, as a practical matter, some data bases are finely partitioned along one variable (e.g. industrial category) and others along another (e.g. plant location), a number of data bases often had to be combined or used in series to determine an activity's distribution.

It should be noted that the Residual Allocation Model and the peripheral air and water models are *comparative* as opposed to *predictive* models. Reliable predictions of absolute pollution levels which will result from various energy strategies are extremely difficult, if not impossible, to make on the basis of currently available information. Accordingly, the model's results are valid only to the extent that they provide a means of comparison between the forseeable impacts that different scenarios can be expected to have on the environment or between the relative environmental impacts of a single scenario on different regions in the analysis.

Residual Allocation Model

The allocation of energy production and associated residuals is performed by two computer models, called the Supply Model and the End Use Model. As their names suggest, the Supply Model allocates the production and residuals directly corresponding to the extraction and refinement of energy resources, whereas the End Use Model allocates the activities and residuals associated with the consumption of these resources for various end uses. Because the most current and complete data is available for 1972, that year is taken as the base year for the projections made by the present models. The models' target year for the Project Independence Blueprint[3] is 1985.

The geographical format of the allocation consists of disaggregating energy production and residuals, predicted on a broad geographical scale by the PIES model, down to the scale of 335 River Basins, defined by the National Oceanographic and Atmospheric Administration, and 243 Air Quality Control Regions (AQCR's), defined by the EPA. The production and residuals assigned to these smaller levels are then available for reaggregation up to the larger regions necessary for analysis of a wider scope.

In the Supply Model, the residual allocation scheme is based on the known location and production of natural energy resources, as well as the location and capacities of existing or planned conversion facilities. Specifically, the allocation proceeds according to the following rules:

1. Production and residuals from existing coal mines which were active in 1972 are allocated on the basis of 1972 production levels.

2. Production and residuals from coal mines predicted to come onstream by 1985 are allocated according to the size, type, and location of known coal deposits.

3. Production and residuals associated with oil and natural gas production and the extraction of oil from oil shale are allocated on the basis of known reserves.

4. Production from coal gasification and liquefaction is assigned on the basis of the sizes and locations of proposed plants.

5. Power plant and refinery activity is allocated according to the location and capacities of facilities projected to be onstream in 1983.

The form of the allocation is quite simple: for each energy activity, the amount of residual k allocated to River Basin (AQCR) j is

$$R_{kj} = \left(\frac{S_j}{S_i} E_i \right) \cdot M_{ki} ,$$

where S_i is the 1972 level of a surrogate quantity associated with the activity in PIES region i containing River Basin (AQCR) j, S_j is the 1972 level of that surrogate in River Basin (AQCR) j, E_i is the forecasted level of the activity in PIES region i; and M_{ki} is the coefficient, specific to region i, of the amount of residual k generated per unit of activity[4]. The choice of surrogates is dependent upon the availability of measures well correlated to the activity, for which data can be obtained reliably at the geographic level required. Once the residuals for each activity have been assigned to River Basins or AQCR's, the model sums the levels of each residual over all activities, thereby arriving at the total River Basin and AQCR loadings for all residuals[5].

The End Use Model follows essentially the same scheme. Activity levels in this segment of the Allocation Model refer to fuel consumption forecasts for various fuels grouped by use categories. The PIES model generates forecasts for these fuel consumption levels for each Demand Region defined by the Census Bureau. The 11 categories treated by the PIES model are:

Industrial Sector	Transportation Sector
Coal	Gasoline
Natural Gas	Jet Fuel
Distillate Oil	Distillate Oil
Residual Oil	Residual Oil

Residential and Commercial Sector
- Natural Gas
- Distillate Oil
- Residual Oil

The variety of activities included in the consideration of end use patterns is extensive, and for most of these activities no comprehensive fuel consumption data are readily available. As a consequence, many different surrogates had to be tabulated in order to effect the disaggregation of consumption levels to River Basins and AQCR's. The End Use Model currently uses the following surrogates:

Fuel Category	Surrogates (1972 data)
All Industrial Fuels	Number of employees in each major industry category. State fuel consumption by 2-digit SIC. National fuel consumption by 4-digit SIC.
Gasoline	State consumption data and population.
Jet Fuel	Number of jet takeoffs.
Transportation Distillate	Primary rail track mileage, interstate highway mileage, population, and vessel bunkering data.
Transportation Residual	Residual consumption at U.S. ports.
All Residential and Commercial Fuels.	Population.

Although more appropriate measures of these consumption levels exist, none were found that were reliable and available at the geographic level required.

After the disaggregation phase, the model converts the consumption predictions into residual loadings for the six air pollution parameters using a set of end use pollutant coefficients developed for fossil fuels[6]. (No water or land use residuals were considered since the only direct environmental impact of the end uses of energy is on air quality.) The output then consists of total levels for each of 6 air residuals in every River Basin and AQCR[7].

As with any model, the Allocation Model depends on several specific assumptions and limitations in scope. One of the most critical of these is the assumed level of pollution control technology. In converting 1985 production and consumption levels to residual loadings predictions, the PIES model supposes that existing and promulgated control standards are enforced and that surface mine reclamation laws will be implemented. Table 1 compares the effect of control technology on the loadings associated with energy supply for one scenario. Moreover, in allocating the new facilities required for the realization of specific scenarios, the model assumes that facility siting patterns will obey the distribution defined by facilities projected to be onstream in 1983. This assumption is consistent with the objectives set forth in the Non-Significant Deterioration legislation now under consideration. Of course, the model also contains the inherent assumptions involved in the use of surrogate quantities for the disaggregation and the suppositions regarding economic and demographic development that are imposed by the choice of 1972 as the base year.

Table 1

EFFECT OF CONTROL TECHNOLOGY[a]

WATER POLLUTANTS

	ACIDS (tons/day)	BASES[b] (tons/day)	TDS (100 tons/day)	SS (tons/day)	ORGANICS (100 tons/day)	THERMAL[c] (E9 Btu/day)
AS/911 with 1972 Control Technology	1,453	23.30	531.5	14,389	5.97	35,384
AS/911 with Advanced Control Technology	0	36.67	50.0	365	1.81	34,021
Major Regulated Activities[d]	Coal mining	Coal mining	Surface coal mining	Coal mining	Oil refining Oil production Coal power generation	Electricity generation

AIR POLLUTANTS

	PARTICULATES (tons/day)	NO(X) (tons/day)	SO(X) (tons/day)	HC (tons/day)	CO (tons/day)	ALDEHYDES (tons/day)
AS/911 with 1972 Control Technology	3,049	82,525	100,369	39,942	9,704.6	198.52
AS/911 with Advanced Control Technology	2,056	33,682	48,317	30,379	1,169.5	391.13
Major Regulated Activities	Coal power generation Oil refining	Fossil fuel power generation	Coal power generation Oil refining	Oil refining	Oil refining Coal power generation	

LAND USE

	SOLIDS (1000 tons/day)	FIXED LAND (100 acres)	MAX. INCREMENTAL LAND (100 acres)
AS/911 with 1972 Control Technology	1,692.9	367,351	21,910
AS/911 with Advanced Control Technology	901.2	356,210	21,460
Major Regulated Activities	Surface coal mining		Surface coal mining

[a] Loadings are for the same amount, type and location of energy activities. In this case the 1985 AS 911 scenario was used.

[b] Effective control of acids from coal mining assumed for advanced technology to accomplished through neutralization with bases.

[c] E9 is 1,000,000,000.

[d] Activity whose regulation causes major loading reduction.

The Allocation Model does not attempt to disaggrate the loadings in curies expected to result from the mining, processing, reprocessing, and waste management associated with the uranium fuel cycle. Curies are a measure of the activity of radionuclides, and as dimensions of residual loadings they do not indicate accurately the quality of radiation in terms of human health risks. Furthermore, the pollution loadings which are analyzed include only those directly attributable to the extraction, processing, conversion, and end use of energy resources, i.e. those which can be quantized per unit of energy in some reasonable fashion. This restriction excludes from the model's scope any pollutants resulting from the construction of energy facilities or from secondary development induced by the exploitation of energy resources. Finally, the model does not take into account pollution loadings, such as spills from pipelines, trains, tankers, etc., that result from the transportation or transmission of energy. The End Use Model does account, however, for vehicle emissions associated with the transport of fuels.

Water Use Model

Ideally, a model to indicate energy impacts on ambient water quality would provide the basis on which to evaluate scenario water use implications. Unfortunately, the physical and chemical dynamics of hydrological phenomena occur on such a small scale that nationwide and even basin-wide predictions of water quality are hardly possible. A river which is anaerobic 30 yards downstream from a paper mill can rid itself of a significant amount of BOD in 30 miles, defying any analysis which looks no closer than the River Basins used for this model. Because of this difficulty of scale, a model to predict water use patterns was developed instead.

The Water Use Model uses an accounting scheme to assess the impacts of scenario-related energy development on water use patterns. The model consists of two sections. The first takes as input the energy production levels predicted by the Supply Model and from these computes energy-associated water withdrawal and consumption for each River Basin. The second section evaluates the resulting energy use predictions in relation to the amount of water available for energy-associated activities (i.e. total water supply minus non-energy use).

More specifically, once all relevant energy activity levels are known for every River Basin, the model converts them to water demand estimates using a set of water use coefficients[8]. Summing the results of this conversion over all energy activities within a basin gives the total energy-related withdrawal and consumption of water for that River Basin. The total water available for all uses in each region is just the sum of inflows from other watersheds, groundwater supply, and indigenous supply from natural runnoff, minus exports to other regions. The water available for energy use is then simply the total water available minus non-energy associated water consumption[7].

Air Quality Model

Although comparison of air pollution loadings among scenarios provides a useful means for evaluating major environmental impacts on a geographical basis, the comparison of the effects these loadings will have on ambient air quality is much more meaningful to decision makers. Unlike hydrological phenomena, atmospheric mixing occurs on a large enough scale to enable rough estimates of the general air quality in the AQCR's. In order to accomplish such an analysis, the Air Quality Model relates 1972 air quality to emissions and then applies this relationship to the emissions predicted for a given scenario. Using such a process, comparisons may be made among scenarios of their relative impacts on regional air quality.

Input to the Air Quality Model consists of energy-associated emissions generated in AQCR's by the Residual Allocation Model for particulates and SO_x. (The lack of adequate monitoring data to evaluate 1972 air quality for other pollutants precluded their consideration.) The model converts the emissions for a single AQCR to an air quality measure and range using conversion factors based on the ratio of indices of 1972 quality to 1972 emissions data. The indices of 1972 air quality are generally the minimum, median and maximum of the 1972 average annual concentrations for all monitoring stations in each AQCR. However, since not all AQCR's were monitored for both pollutants in 1972, some of the data used in the present model are taken from 1974 data, or, in some cases, from data for AQCR's judged to possess similar topographic, atmospheric, demographic, and industrial characteristics.

The crucial assumption in the Air Quality Model is that the relationship between emissions and ambient quality is linear and time independent in every AQCR. This is justifiable only insofar as no drastic changes occur in the distribution or overall quantity of particulates and SO_x emitted between 1972 and 1985. It also requires that each AQCR experience no drastic climatological changes during the interim. Moreover, because the analysis is conducted on a basin-wide scale, no distinction is made between point and area sources of residuals or between stack heights at which pollutants are emitted. Site-specific air quality models cannot be applied in this context because projections of the location of energy activities cannot be accurate beyond the AQCR level. At this point in time, attempts at formulating a more precise functional relationship between emissions and quality are also hampered by the fact that monitoring of emissions and air quality only now approaches a comprehensive network. Until a substantial history of comprehensive monitoring in all AQCR's becomes available, roll-back approximations like that used in the Air Quality Model will be the best empirical relationships obtainable for this level of analysis. For this reason, it is imperative that the output of the model be used for comparison purposes only. The air quality estimates do not necessarily provide realistic predictions of 1985 air quality. However, since the same analysis is used regardless of the scenario being considered, the model is useful as a basis for comparison among scenario impacts on air quality[7].

Conclusions and Recommendations

The results of the model are useful for comparison of the environmental impacts of energy alternatives and as indicators of specific regions needing further study on the effects of energy development. The output cannot be used as a *definitive* indicator of environmental "hotspots." The major conclusion drawn from the analysis performed up to now stems from the model's sensitivity to assumptions regarding pollution control technology. The degree to which control technology will be implemented between now and 1985 is the single most influential factor of the impacts which various scenarios exert on the environment.

Most of the important general limitations of the model have been outlined earlier. The model is clearly not site-specific in its methodology; the allocation of residuals goes no further than the River Basin level, with no explicit consideration of topography, climate, or severity of particular point sources. The model also inherits all of the limitations of its various inputs, including the PIES Model output, the residual and water use coefficients, and the data taken from the many other sources. Another crucial concept whose limitations must be taken into account is that of a "residual." The fifteen residuals allocated by the model define relatively broad *classes* of environmental impact. For example, predictions of loadings in organics, measured in hundreds of tons per day, do not distinguish between chemically different hydrocarbons. Loadings estimates for solids, measured in thousands of tons per day, lump together all residuals which do not enter the air or water. They include such different wastes as spent shale from oil shale processing and scrubber sludge from coal-fired power plants. Residuals provide a convenient, allocable set of impact categories by which the overall effects of energy development can be compared.

Several areas needing further study or attention have become evident through the development and application of the Residual Allocation Model. There is an obvious need for more extensive environmental monitoring. Also, if energy planning is to advance, better regional census data must be gathered. Much of the uncertainty imposed by the use of surrogates could be mitigated if a more complete inventory of regional and local energy consumption patterns were available. A sensitivity analysis of the model should be conducted to include variations in the method of projecting facility siting, along with an investigation into the degree of control technology that one realistically can expect to be implemented by 1985.

The analysis should be expanded to include at least three additional areas of environmental impact. To begin with, some assessment ought to be made of the ramifications of facility construction on surrounding areas. The construction of water-diverting facilities for a hydroelectric plant, for example, may take ten or more years. The resulting temporary and long-term changes in the surrounding water quality are not included in the present model. Further study should also be conducted into the possibility of presenting radioactivity and trace metal loadings on a regional basis in terms that relate to potential human health hazards. Finally, it might be useful to introduce an energy accounting scheme which would examine Btu production and consumption on both the regional and national levels. Such a program would indicate the relative energy productivity and demand distributions among River Basins or AQCR's and would help measure the degree of environmental damage export. The output of the model then could be used to examine the questions of who is producing the energy for whom and at what environmental cost.

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HITTMAN REGIONAL ENVIRONMENTAL COEFFICIENTS FOR THE PROJECT INDEPENDENCE EVALUATION SYSTEMS (PIES) MODEL

Matthew S. Mendis, Jr.
William R. Menchen
H. Lee Schultz, III
Energy Systems Department
Hittman Associates, Inc.
Columbia, MD

Summary

The development and utilization of environmental coefficients for the environmental/policy analysis of energy strategies is described in this paper. The paper outlines Hittman Associates' efforts as a member of the Project Independence Blueprint Environmental Task Force. The extensive environmental data bank developed for the Project Independence Evaluation Systems (PIES) model is described along with its utility in the policy analysis decision stream. The limitations of the data bank are discussed, and suggested modifications recommended. The technique for determining environmental residuals as accomplished by the PIES Environment Report is also described. The conclusion is that the Hittman environmental coefficients can be utilized effectively in a first-cut comparative environmental analysis of energy scenarios.

Introduction

The Hittman Regional Environmental Coefficients were developed for the environmental analysis of the Project Independence Blueprint (PIB). The purpose of PIB was to analyze the economic, environmental and social impacts of different possible Government policies on future energy supply and demand. In order to achieve this, the Federal Energy Administration, in an interagency effort, developed the Project Independence Evaluation Systems (PIES) model to forecast energy supply and demand for different sets of assumed government policies and imported oil prices. Attached to the PIES model was an "Environment Report" submodel which was developed by the Environmental Cross-Cut Task Force headed by the Environmental Protection Agency (EPA).

As a member of the PIB Environmental Task Force, Hittman Associates, Inc. (HAI) was assigned the task of: 1) defining the environmental indicators to be used in the energy assessment; 2) establishing the environmental data requirements; 3) defining the pollution abatement technologies; 4) identifying environmental constraints to be included in the price equilibrium mode; and 5) developing environmental data for quantitative analysis of each of the PIES generated scenarios.

The principal and most important task was the development of regional environmental coefficients for the quantitative analysis of PIB. To accomplish this task, HAI aggregated into the PIES model an extensive environmental data bank previously developed under contract with the Council on Environmental Quality[1]. Where necessary, the earlier coefficients were updated and revised or new coefficients developed. The coefficients represent units of pollutants (i.e., air and water pollutants solid waste, land use and occupational health) per unit of energy supplied, converted or consumed. The environmental coefficients were also regionalized according to the energy activity considered. For example, environmental coefficients for coal supply were developed for the twelve coal supply regions shown in Figure 1. The regional coefficients reflect variations in the characteristics of the energy resource, extraction, processing, storage and utilization.

The environmental coefficients developed for the PIB were integrated into PIES as a subprogram. The subprogram utilizes the output of the supply/demand portion of PIES and the Hittman Regional Environmental Coefficients to generate the PIES Environment Report. This report presents the environmental residuals (i.e., total quantity of each pollutant) associated with each energy supply, conversion and end use activity. The environmental residuals were determined by taking the product of the level of an energy activity (i.e., tons of coal supplied per day) and that energy activity's environmental coefficients (i.e., lbs of pollutant per ton of coal supplied). A flow diagram of the Environment Report algorithm is presented in Figure 2.

A generalized discussion of the Hittman Regional Environmental Coefficients is presented in the following sections. A detailed presentation of these coefficients is available in Reference 2.

Data Development

Basis for the Environmental Coefficient Matrices

The basic references used in preparing the environmental coefficient matrices supplied to the FEA Project Independence model were two reports prepared by Hittman Associates for the Council on Environmental Quality (CEQ) on the environmental impacts, efficiency, and cost of energy supply and end use.[1] These reports, issued in final November 1974, presented quantified data on the broad range of environmental impacts to land, water, and air for each step in the fossil fuel supply and end use chain. The reports covered the fossil fuel supply system components, all electric power plant conversion for coal, oil, and natural gas and some of the future supply activities including high and low Btu coal gasification, oil shale, and coal liquefaction. New data was obtained by HAI for the nuclear fuel cycle, hydroelectric power plants, transportation of energy resources and energy end use (transportation, residential/commercial, and industrial) activities.

The format of the data presented in the CEQ reports was at a lower level of aggregation than that required for the Project Independence model. Since the CEQ impact data was derived for each step in the energy supply trajectory, it was necessary to aggregate the environmental impacts from several steps in order to arrive at a set of coefficients consistant with the level of aggregation specified in the PIB model. Also, the CEQ data is presented in terms of impacts per trillion Btu input to each process, and it was desired to put these impacts on a physical units basis (tons of coal, bbl of oil, etc.) to be consistent with the energy flow format of the PIB model.

Coal production provides an illustrative example. The PIB model specifies the tons of coal produced, ready for shipment, from each of twelve coal supply regions. To get to this point, several unit operations or activities must be performed on the coal resource in the ground. First the coal must be extracted. It must then be transported locally to a preparation site and stored. It may then be prepared by washing to remove impurities or just sized for shipment. Each of these activities may, in turn, be performed by one or more specific processes. Extraction of coal in the Hittman data base is comprised of underground (room and pillar, and longwall) and surface (auger, strip, and contour) mining techniques or processes. Local transportation of the coal can be performed by mine rail, conveyor, or trucks. Preparation of the coal may involve washing (dense media) or simple breaking and sizing.

As a concrete illustration of the methodology employed to manipulate the Hittman data for use with the PIB model, consider coal production from existing underground mines in Northern Appalachia. From Bureau of Mines' data for this region it was determined that 75 percent of the coal extracted from the ground received some type of mechanical cleaning and that the remaining 25 percent was just mechanically crushed or sized. Bureau of Mines' data further showed that 95 percent of the coal from this region was extracted by room and pillar operations, while 5 percent was extracted by the longwall method. These relative fractions were the basis for determining the combination and weighting of processes used from the data base.

The procedure used was to work backward from the point of coal ready for shipment and determine, using the respective process efficiencies, the Btu input needed to deliver this amount of coal. The Btu input numbers (recall that the data base is on a trillion Btu input basis) represent the multipliers used with the data base environmental coefficients to determine the environmental impact from that respective operation. A summation of impacts over all operations then gives the coefficients for use with the PIB model. Table 1 and Figure 3 illustrate the derivation of one (of 18) PIB environmental coefficients for underground coal production from the Northern Appalachian region.

Table 1. Derivation of PIES Coefficient From CEQ Data

	Data Base Solid Waste Impact/ 10^{12} Btu Input	Btu Input Multipliers	Tons Solid Waste per 10^{12} Btu
Room and Pillar Extraction	1.19+03	1.71	2.03+03
Longwall Extraction	1.78+03	.06	1.07+02
Mine Rail Transport	0	1.028	0
Steam Coal Preparation	5.97+03	.778	4.64+03
Breaking and Sizing	2.54+00	.25	6.35-01
		Total =	6.78+03

$$\frac{6.78{+}03 \text{ tons solid waste}}{10^{12} \text{ Btu for delivery}} \times \frac{10^{12} \text{ Btu}}{42.4\text{x}10^{3} \text{ tons coal}} = \frac{1.59{+}02 \text{ tons solid waste}}{10^{3} \text{ tons coal for delivery}}$$

Additional data were obtained through a literature search for those energy activities not included in the CEQ report. Specifically, environmental matrices were developed independent of the CEQ report for the nuclear fuel cycle, hydroelectric power plants, energy transportation, and all the end use activities.

Data Format

The Hittman environmental data was designed to facilitate its incorporation and utilization in the PIES model or any other similar energy model. Environmental coefficients are given on the basis of unit of pollutant produced per unit of energy input or output associated with an energy activity. For example, the nitrogen oxides (NO_x) associated with the extraction of natural gas was determined to be $2.75\text{x}10^{-3}$ tons NO_x per 10^6 SCF natural gas. Thus, if a region produces $250\text{x}10^6$ SCF of natural gas per day, the associated environmental residual can be determined as:

$$\left(250\text{x}10^6 \frac{\text{SCF}}{\text{day}}\right) \times \left(2.75\text{x}10^{-3} \ \frac{\text{tons } NO_x}{10^6 \text{ SCF}}\right)$$

$$= 6.875\text{x}10^{-1} \text{ tons} \frac{NO_x}{\text{day}}$$

The environmental data for each energy activity is presented in a matrix where the energy activity and regions make up the rows and the environmental pollutants make up the columns. An example matrix can be found in Figure 4.

A discussion of the energy activities, the environmental pollutants and the regional delineations that make up the Hittman Environmental Coefficient Matrices is presented below.

Data Description

Definitions

In order to describe the environmental impacts associated with energy supply, conversion and end use, a number of definitions were adopted:

Term	Example/Definition
Pollutant	SO_2 emission from the combustion of coal for steam generation
Process	Combustion of coal for steam generation (results in a set of pollutants)
Activity	A combination of processes (i.e., electricity generation by coal-fired power plants)
Environmental Coefficient	Unit of pollutant per unit of energy into an activity (i.e., lbs of SO_x emitted per ton of coal into a coal-fired power plant)

Environmental Residual	The total quantity of a pollutant for a given time period resultant from an energy activity (i.e., tons of SO_x emitted per day)

Controlled Vs. Uncontrolled

All environmental coefficients incorporated in the PIES model were designated controlled. "Controlled" implies that impacts are consistent with the use of control technology which will probably be required and/or available in 5 to 10 years. As an illustration, past laws that governed the reclamation of surface mined lands minimally required that effort be made to restore the land. This included partial backfilling and an attempt at revegetation. However, since the degree and success of reclamation were not mandatory, (for the "uncontrolled" condition) reclamation was not assumed for area stripping operations, and only partial backfilling was assumed for contour mines. In the controlled situation, contour backfilling and revegetation were assumed required for either type of stripping operation. The attainment of this high level of reclamation will require such practices as stockpiling and redistribution of the topsoil, segregation of toxic overburden, and seed bed preparation. Generally speaking, the controlled condition incorporates the environmental standards proposed or soon to be implemented by the EPA. A more detailed explanation of controlled as it is related specifically to each process in the energy activity chain is to be found in the writeups preceding each energy activity environmental matrix in Reference 2.

Uncontrolled environmental coefficient matrices were developed for comparison of a "base case" to the PIES scenarios. "Uncontrolled," according to the ground rules adopted in this study, means that impacts are the current national or regional average value. In the absence of current (1972-73) data, impacts typify the use of least stringent environmental controls. The uncontrolled environmental coefficients are not presented in Reference 2. However, uncontrolled environmental coefficients in the CEQ format are presented for fossil fuel energy activities in Reference 1.

Energy Activities

The energy related activities evaluated for environmental residuals in the PIES data base were:

- Coal Supply:
    - Underground
    - Surface
- Coal Gasification:
    - Low Btu
    - High Btu
- Coal Liquefaction
- Shale Oil Supply:
    - Underground
    - Surface
    - In-Situ
- Natural Gas Supply:
    - Extraction
    - Processing
- Crude Oil Supply:
    - Domestic Onshore
    - Domestic Offshore
- U_{235} Extraction
- Energy Transportation:
    - Coal:
        - Railroad
        - Barge
        - Pipeline Slurry
    - Crude & Syncrude Oil:
        - Pipeline
    - Crude Oil:
        - Barge
        - Railroad
    - Crude & Refined Oil:
        - Tanker
    - Oil Products:
        - Barge
        - Truck
        - Rail
        - Pipeline
    - Natural & Synthetic Gas:
        - Pipeline
    - Liquefied Natural Gas:
        - Tanker
    - Deep Draft Port Facility:
        - Monobuoy Mooring System
- Power Plants:
    - Coal Fired
    - Oil Fired
    - Gas Fired
    - Gas Turbine Simple Cycle
    - Low Btu Gas/Steam Turbine Combined Cycle
    - Hydroelectric
    - Nuclear
- Electricity Transmission & Distribution
- Oil Refineries
    - Existing
    - New - (Fuel Oil)
    - New - (Gasoline)
- Transportation Energy End Use
- Residential/Commercial Energy End Use
- Industrial Energy End Use

The energy activities analyzed for environmental residuals are only those directly attributable to energy material extraction, processing, and utilization on a per unit of energy basis. Because residuals from other energy-related activities cannot be estimated on the basis of a per unit of energy input or output, environmental coefficients were not developed for pollutants resulting from:

- Construction of energy facilities
- Conjunctive development induced by energy development
- Secondary pollutants resultant from interaction of primary pollutants with the environment

Environmental Pollutants

The environmental pollutants considered in the PIES data base were:

- Water Pollutants:
  Acids, Bases, Total Dissolved Solids, Suspended Solids, Organics, Thermal
- Air Pollutants:
  Particulates, Nitrogen Oxides, Sulfur Oxides, Hydrocarbons, Carbon Monoxides, Aldehydes
- Land Impacts:
  Solid Waste, Permanent Land Use (Fixed Land), Temporary Land Use (Maximum Incremental Land)
- Occupational Health:
  Deaths, Injuries, Man-days Lost

The water and air pollutants are aggregated in broad categories such as acids, bases, particulates, etc. The constituent pollutants (i.e., sulfuric acid, calcium carbonate, trace metals, etc.) are not identified for two reasons. First, the time allocated for development of the environmental coefficients for PIES precluded any further breakdown. Secondly, the level of information on the energy activities generated by PIES was such that accuracy would not be enhanced if any further breakdown in the pollutant categories was attempted. The broad pollutant categories had the advantage of facilitating qualitative environmental analysis of the PIES scenarios.

Solid wastes are considered to be all residuals not entering the air or water that result from the basic fuel resource, or from the system processes that make fuels useful for consumption.

The land impacts include areas required for extraction, structures, disposal of solid wastes, roads, ports, pipelines, storage, and buffer zones. Both fixed and incremental land effects are considered. Fixed land effects are those associated with facilities such as processing plants, pipelines and storage tanks, whereas incremental land effects are those associated with excavation, such as strip mining, and solid waste disposal.

Occupational health is considered on the basis of deaths, injuries, and man-days lost due to injuries.

Regionalization

In order to be compatible with the PIES output, environmental coefficients for each energy activity were determined regionally to reflect variations in the characterization of the energy activities. PIES regions for each energy activity were defined to "correspond to natural data divisions appropriate to each resource, conversion facility and demand."[3] The results of this regional division are shown in Table 2.

Table 2. PIES Energy Regions

Energy Activity	Number and Region Definition
Coal Supply High Btu Gasification Low Btu Gasification Coal Liquefaction	12 FEA Coal Supply Regions (See Figure 1)
Oil Production Natural Gas Production Natural Gas Processing	14 NPC Petroleum Provinces of the U.S.
Energy Transportation	National
All Electric Generating Power Plants	9 Census Regions
Oil Refineries	7 Petroleum Administration for Defense (PAD) Districts
Oil Shale Recovery U-235 Extraction Electricity Transmission and Distribution	National
Residential/Commercial End Use Industrial End Use Transportation End Use	9 Census Regions

Environmental coefficients were developed for the PIES regions utilizing a weighting system to reflect the variation within a given region of:

- Energy resource characteristics
- Energy production, conversion and utilization
- Regulatory requirements on energy supply, conversion and end use (i.e., environmental constraints)
- Energy consumption patterns

Environmental Coefficient Matrices

The result of the HAI/PIES effort was the development of a comprehensive set of environmental coefficient matrices for energy supply, conversion and end use. Thirty-three matrices were developed encompassing the energy activities, pollutants, and regions discussed above. These environmental matrices, the associated assumptions, the methodology for their utilization and a sensitivity analysis are presented in Reference 2.

Data Application

General

The Hittman Regional Environmental Coefficients developed for the PIES model have potential for a wide range of applications. The present format of units of pollutant per unit of energy input or output has the advantage (over the CEQ format of 10^{12} Btu's into a system) of compatible application to most existing data bases. The use of consistent environmental coefficients also enables energy policy makers to obtain relative environmental rankings of various energy strategies. The regional characteristics of most of the coefficients allow for the focusing of environmental analysis to specific regions without a loss of resolution. Environmental coefficients and the subsequent environmental residuals analysis has the advantage of allowing the comparison between energy alternatives without getting into the site specific nature of the energy facilities. Thus, it becomes possible to discuss representative energy activities rather than specific facilities (i.e., a particular power plant). Additionally, the residual analysis has a further advantage in that it is required as a primary step if one wants to proceed to an environmental quality analysis and subsequent environmental impact assessment.

Application to PIES

The output of PIES for the Environment Report is a series of energy activity levels relating to energy supply, conversion, transportation and end use within a given region. The environmental evaluation of each PIES scenario requires explicit consideration of the entire set of energy activities and the environmental residuals that are generated by these activities. The Hittman Environmental Coefficients, as utilized in PIES for residual analysis, are described below.

Consider the following: i energy activities; j regions; and k environmental pollutants. Then we can define the following:

E_{ij} = the level of the ith energy activity in the jth region

P_{ijk} = the kth environmental coefficient for the ith energy activity in the jth region

Utilizing the definitions above, we can determine various aggregations of environmental residuals (ER) as is done in PIES by the following operations:

$ER_{ijk} = E_{ij} \times P_{ijk}$: the residuals associated with a regional energy activity

$ER_{jk} = \sum_i (E_{ij} \times P_{ijk})$: the residuals associated with all regional energy activities

$ER_k = \sum_i (\sum_i (E_{ij} \times P_{ijk}))$: the residuals associated with total national energy activities

The procedure of product summations to determine environmental residuals allows for incorporation into other regional or national energy models.

Conclusions and Recommendations

The immediate conclusion is that the Hittman environmental coefficients can be utilized as an effective tool in the policy analysis of energy strategies. The relative environmental residuals comparison of various energy strategies can aid in pointing out environmental problem areas of future energy development. The environmental residuals technique allows for a rapid, broad analysis of energy strategies and can indicate those strategies or regions that should be studied in more depth. However, the environmental residuals technique can be utilized only as a means of comparison between strategies, and not as a statement of environmental quality.

Several recommendations for refinement of the environmental coefficients technique can be identified. These include:

(1) Development of additional environmental coefficients for pollutants not considered in PIES such as specific trace metals, etc.

(2) Consideration of secondary pollutants that result from the interaction of primary pollutants with the environment

(3) Development of techniques to reflect residuals that are time variant with energy throughputs (i.e., acid mine drainage, reclamable land use, radioactive waste, etc.).

(4) Development of more uniform regions so as to optimize coefficient resolution within the available data base

(5) Finally, better techniques should be developed to utilize the residuals data for a generalized environmental quality analysis (i.e., building in quality indicators for each type of pollutant in order to reflect the sensitivity of any given region to an increase in a given environmental residual)

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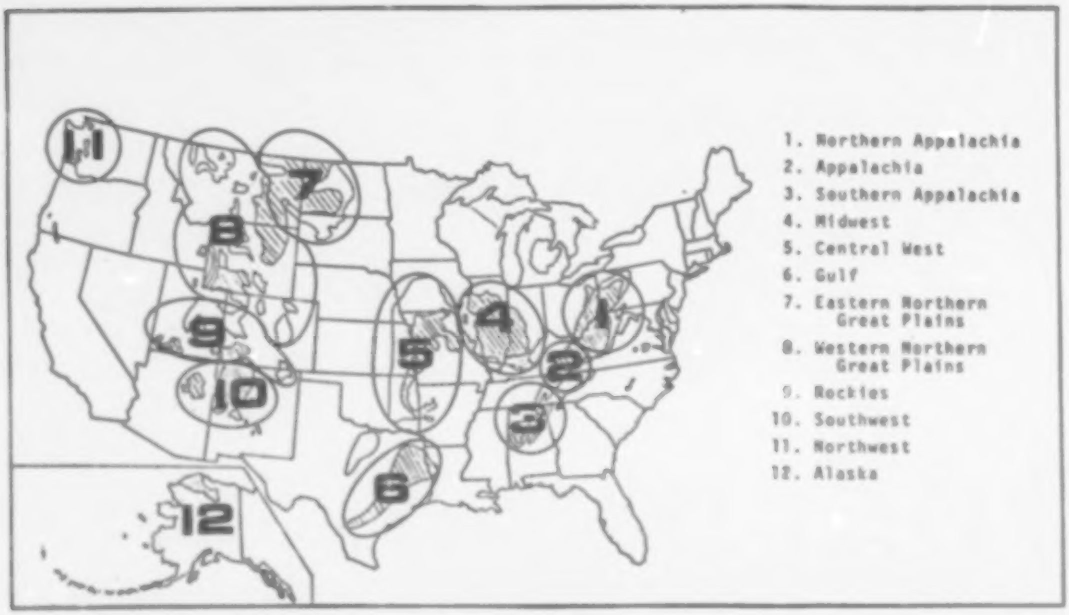


Figure 1. PIES Coal Supply Regions

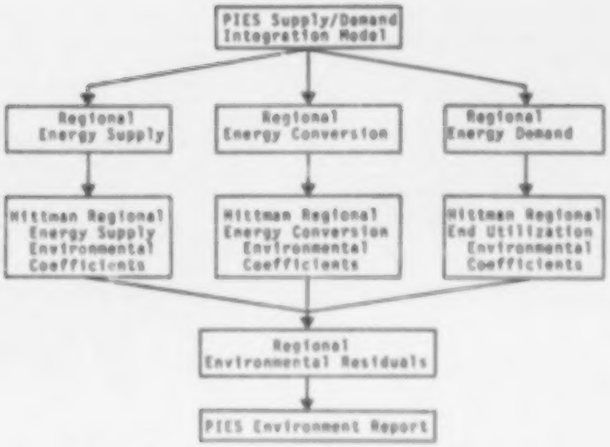

PIES Supply/Demand Integration Model
Regional Energy Supply
Regional Energy Conversion
Regional Energy Demand
Hittman Regional Energy Supply Environmental Coefficients
Hittman Regional Energy Conversion Environmental Coefficients
Hittman Regional End Utilization Environmental Coefficients
Regional Environmental Residuals
PIES Environment Report

FIGURE 2. Environment Report Generation

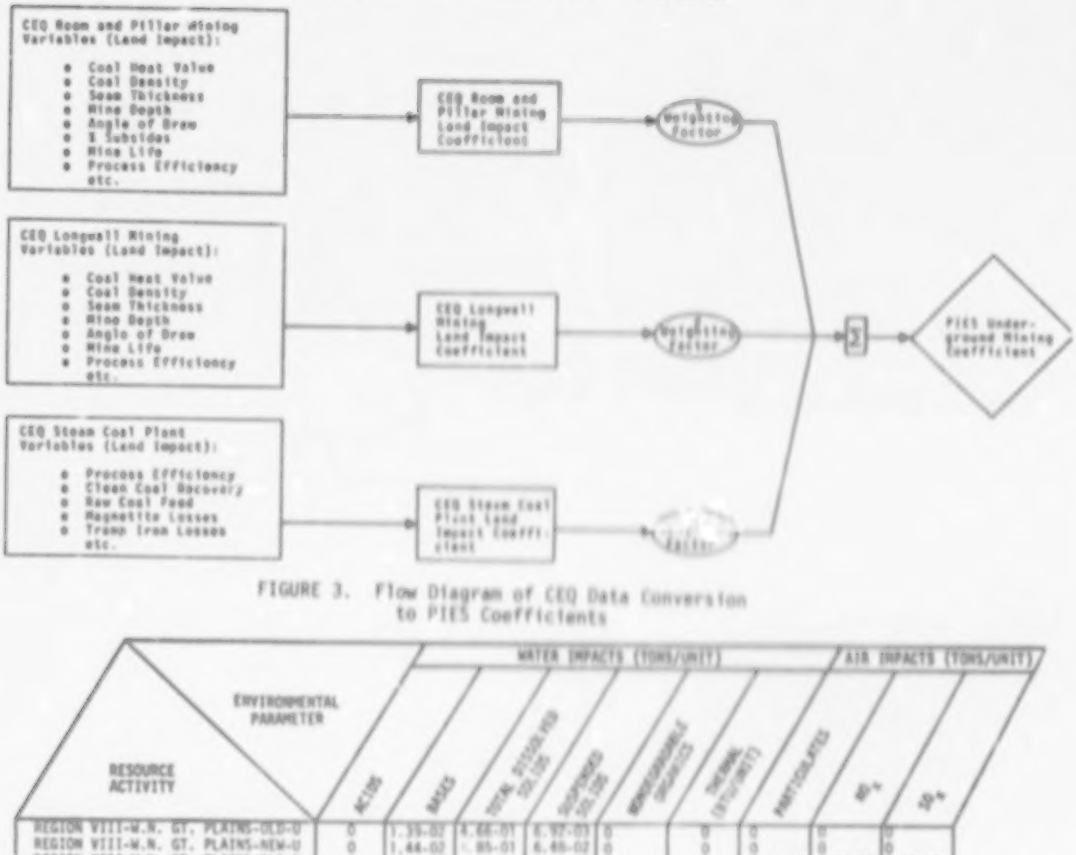

CEQ Room and Pillar Mining Variables (Land Impact):
● Coal Heat Value
● Coal Density
● Seam Thickness
● Mine Depth
● Angle of Draw
● % Subsides
● Mine Life
● Process Efficiency etc.
CEQ Room and Pillar Mining Land Impact Coefficient
Weighting Factor
CEQ Longwall Mining Variables (Land Impact):
● Coal Heat Value
● Coal Density
● Seam Thickness
● Mine Depth
● Angle of Draw
● Mine Life
● Process Efficiency etc.
CEQ Longwall Mining Land Impact Coefficient
Weighting Factor
CEQ Steam Coal Plant Variables (Land Impact):
● Process Efficiency
● Clean Coal Recovery
● Raw Coal Feed
● Magnetite Losses
● Tramp Iron Losses etc.
CEQ Steam Coal Plant Land Impact Coefficient
Factor
Σ
PIES Underground Mining Coefficient

FIGURE 3. Flow Diagram of CEQ Data Conversion to PIES Coefficients

ENVIRONMENTAL PARAMETER / RESOURCE ACTIVITY	WATER IMPACTS (TONS/UNIT)						AIR IMPACTS (TONS/UNIT)		
	ACIDS	BASES	TOTAL DISSOLVED SOLIDS	SUSPENDED SOLIDS	NONDEGRADABLE ORGANICS	THERMAL (BTU/UNIT)	PARTICULATES	NO_x	SO_x
REGION VIII-W.N. GT. PLAINS-OLD-U	0	1.35-02	4.66-01	6.92-03	0	0	0	0	0
REGION VIII-W.N. GT. PLAINS-NEW-U	0	1.44-02	4.85-01	6.48-02	0	0	0	0	0
REGION VIII-W.N. GT. PLAINS-OLD-S	0	0	0	0	0	0	1.64-02	2.74-02	2.02-03
REGION VIII-W.N. GT. PLAINS-NEW-S	0	0	0	0	0	0	1.64-02	2.74-02	2.02-03
REGION IX - ROCKIES - OLD - U	0	1.94-02	6.51-01	4.62-02	0	0	0	0	0
REGION IX - ROCKIES - NEW - U	0	1.97-02	6.62-01	7.65-02	0	0	0	0	0
REGION IX - ROCKIES - OLD - S	0	0	0	0	0	0	6.48-02	2.40-02	1.75-03
REGION IX - ROCKIES - NEW - S	0	0	0	0	0	0	6.48-02	2.40-02	1.75-03
REGION X - SOUTHWEST - OLD - U	0	1.67-02	5.63-01	3.99-02	0	0	0	0	0
REGION X - SOUTHWEST - NEW - U	0	1.70-02	5.72-01	6.62-02	0	0	0	0	0
REGION X - SOUTHWEST - OLD - S	0	0	0	0	0	0	5.61-02	2.07-02	1.51-03
REGION X - SOUTHWEST - NEW - S	0	0	0	0	0	0	5.61-02	2.07-02	1.51-03
REGION XI - NORTHWEST - OLD-U	0	1.44-02	4.83-01	6.48-02	0	0	0	0	0
REGION XI - NORTHWEST - NEW-U	0	1.44-02	4.03-01	6.48-02	0	0	0	0	0
REGION XI - NORTHWEST - OLD-S	0	9.47-03	3.19-01	5.08-02	0	0	1.57-03	4.47-02	3.29-03
REGION XI - NORTHWEST - NEW-S	0	7.72-03	2.60-01	3.86-01	0	0	1.34-03	3.80-02	2.78-03
REGION XII - ALASKA - NEW - U	0	0	0	0	0	0	0	0	0
REGION XII - ALASKA - NEW - S	0	0	0	0	0	0	1.81-03	5.15-02	3.76-03

FIGURE 4. Environmental Coefficient Matrix for Coal Supply

INTEGRATED ECONOMIC-HYDROSALINITY-AIR QUALITY ANALYSIS FOR OIL SHALE AND COAL DEVELOPMENT IN COLORADO

Charles W. Howe
Bernard Udis
Robert C. Hess
Douglas V. Orr
Jeffrey T. Young
Department of Economics
University of Colorado

Jan F. Kreider
Environmental Consulting Services
Boulder, Colorado

Summary

The objective of this study was to analyse the economic, hydrologic, water quality, and air quality implications of establishing a shale oil industry and expanding coal mining in Colorado. The main tools of analysis consisted of (1) the Colorado State University input-output (I-O) model of the State; (2) the University of Colorado (I-O) models of the Upper Main Stem of the Colorado (UMS) and Green River Basin economies; (3) the C.U. hydro-salinity model calibrated to the UMS, White, and Yampa basins; (4) the C.U. air quality model; and (5) state 1970 date on employment by industry and skill, the latter reduced to a set of employment coefficients per million dollars of output for the various sectors of the State economy. The strategy was to analyze three steady-state scenarios: a shale oil scenario, an underground coal mining expansion scenario, and a strip mining coal expansion scenario. Changes in outputs and employment due to oil shale and coal expansion were estimated.

The coal scenario consisted of 6 underground expansions totaling 10.35 million tons per year in the UMS Basin and 5 strip mining operations totaling 12.45 million tons per year in the Green River Basin. The shale oil scenario consisted of 4 operations totaling 134,000 bbls/day in the UMS Basin and 3 operations totaling 146,000 bbls/day in the Green River Basin. The steady-state increase in statewide output levels due to shale oil was about $1.6 billion. Increased payments to households totaled $134 million statewide. The statewide increase in employment was 16,670.

The underground coal expansion induced an expansion in statewide output levels of $171 million, increased payments to Colorado households of $27 million, and direct and indirect increases in employment of 4964 persons.

The strip mining expansion increased statewide output levels $47 million, increased payments to Colorado households by $3.8 million statewide, and increased employment by 1300 persons.

The water implications included direct and indirect consumptive uses of 31,668 acre-feet per year in the UMS, 34,164 per year in the White River Subbasin, and 8520 in the Yampa. Added salt loadings were 3576, 5568, and 3204 tons per year in the 3 basins, assuming that brine and spent shale problems will be totally controlled. Shale oil production is the major air polluter. Some 17 phases of the shale oil process contribute significantly to air pollution. It is predicted that a significant degradation of air quality will occur in Garfield and Rio Blanco Counties from the postulated 280,000 bbl/day industry on the assumption that processes similar to TOSCO II will be used. Occasional conditions of poor dispersion could lead to much more severe short term episodes. Ambient air quality impacts in the vicinity of the plant itself are seen to be critically dependent on plant location with respect to topographic features.

Methods of Analysis

The scenarios analyzed are given below in Tables 1 and 2. They represented the best available estimates of likely developments as of June, 1975. It should be noted that only the direct and indirect efforts of coal and shale oil production have been analyzed. The coal and oil produced have been treated as exports from Colorado, even though some are intended for use within the State.

Table 1.
Coal Scenario

Company/Location	Ultimate Tonnage	Meth-od	Uses
Colorado River Basin			
1. Colo. Consol. (Columbine Glass)Paonia	2.0×10^6	UG	Export from State
2. Adolph Coors Bowie-Paonia	4.0×10^6	UG	To Golden
3. Pittsburgh/Midway Paonia	1.0×10^6	UG	Export from State
4. Atlantic Richfield Somerset	2.0×10^6	UG	Export (?)
5. Western Slope Carbon Somerset	0.6×10^6	UG	To Pueblo
6. Public Service Co. Cameo	0.75×10^6	UG	Thermal, Cameo
TOTAL	10.35×10^6	UG	
Green River Basin			
1. Empire Energy Moffat City	2.0×10^6	S	Slurry Pipe to Texas*
2. Utah International Craig (Moffat C.)	2.6×10^6	S	Thermal, Craig
3. W. R. Grace Moffat County	3.0×10^6	S	Slurry Pipe to Texas*
4. Peabody Routt County	0.85×10^6	S	Thermal, Hayden #2
5. Energy Fuel Routt County	4.0×10^6	S	To Denver
TOTAL	12.45×10^6		

* requires water & power

The basic tool of economic analysis used was in the input-output (I-O) type of model. Excellent expositions of this type of model are available in the literature (e.g. Baumol[1] or Miernyk[2]) but, in brief, such a model shows the linkages which exist among the various economic sectors of a region by virtue of

Table 2.
Shale Oil Scenario

Company/Location	bbls/day	Retorting Tech.[2]	Mining Tech.
Colorado River Basin[1]			
Colony	46,000	TOSCO II	UG
Union	50,000	Union Underfeed	UG
Occidental (Garrett Res.)	30,000	In Situ	--
Paraho	8,000	Paraho	UG
TOTAL	134,000		
Green River Basin			
Superior	50,000	Superior 3 Minerals	UG
Rio Blanco (C-a)	50,000	TOSCO II	UG
Shell Oil (c-b), (formerly ARCO)	46,000	TOSCO II	UG
TOTAL	146,000		

1/ Omitting all Utah developments.
2/ We will assume TOSCO II for all plants.

supplying one another with inputs. The linked sectors include households and a local-state government sector. When one sector expands its output (say to satisfy a new national demand for an energy commodity like coal), it demands more inputs from other economic sectors of the region, and they, in turn, demand more from their suppliers (including households which supply the labor inputs required). Some inputs are imported from outside the region, and such "leakages" finally cause the total regional requirements to converge to new equilibrium levels of output for each regional economic sector.

Should it be desired to know how much of a pollutant will be generated by the regional economy or how much of some natural resource like water will be required, it is then possible to multiply the output levels by corresponding coefficients representing the generation of the waste or use of the resource to arrive at a total. This procedure is followed, for example, in determining non-agricultural consumptive water uses, the total level of wastes generated, and employment by sector. More complex models are needed to determine the water use of agriculture and the patterns by which air-borne wastes are distributed at ground levels.

The regions for which I-O models exist are: the Green River Basin, the Upper Main Stem of the Colorado River (UMS), the San Juan River Basin, and the State of Colorado. The first two were used to represent the economic structures of their respective portions of the State of Colorado. The Green and UMS I-O models were used in conjunction with Gray's I-O model[3] of the entire State to analyze statewide and regional economic effects.

To trace water use in greater detail and to analyze the salinity (total dissolved solids) effects on water quality of the energy developments under study, the hydro-salinity model (Udis, Howe, and Kreider[4]) was calibrated to three separate sub-basins: the Colorado UMS below Glenwood Springs (excluding the Gunnison-Uncompaghre systems); the White River; and the Yampa River. The outputs of the models include monthly and annual river basin outflows, and total dissolved solids loadings by month and year.

The air pollution model does not cover regions but calculates ground level concentrations of particulates, sulphur dioxide, oxides of nitrogen, carbon monoxide, and unburned hydrocarbons for areas surrounding important point and diffuse sources. A point source would be, for example, a coal mine or a thermal electric plant. A diffuse source would be a town where there are many small point and mobil sources.

The strategy of applying these models to the analysis of the coal and shale oil scenarios consisted of the following steps:

1. use the state-wide I-O model to get total state output and employment effects;
2. use the UMS I-O model to get the output and employment effects occurring in the UMS region (roughly Garfield, Mesa, Delta, and Montrose Counties) as a result of the coal and shale oil developments;
3. use the Green River Basin I-O model to estimate the output and employment effects of the coal and shale oil developments assumed for that region (Rio Blanco, Moffat, and Routt Counties);
4. assume that the "rest of the State" effects are given by the quantities in (1) less those in (2) and (3);
5. apply the hydro-salinity models to the immediate basins where the developments are occurring, since that is where any critical water problems will arise;
6. apply the air pollution model to the important new point sources.

For shale oil and the new strip and underground coal mining processes, the major problem was to create the column of technical coefficients showing the inputs from the regional (or state) sectors. Each entry requires two facts: (1) the technologically required input from the particular sector and (2) the portion of that input likely to be supplied by the regional (state) sector (the remainder being the amount imported. It was decided that the rows corresponding to the new energy activities and showing the distribution of their output would all be zeroes, the output being completely exported from the State. (This is not the case for all coal output; see the Coal Scenario in Table 1).

The major sources consulted during the construction of the shale oil column were references 5 thru 10. Reference 11 would have been extremely useful had it been known in time. Interviews with officials of the Shale Oil Corporation provided new information and verification of data from other sources.

The final data used to characterize the oil shale sector were stated in terms of the annual inputs into a 50,000 bbl/day plant, the output of which was evaluated at $12 per barrel. These are given in Table 3.

Table 3.
Major Inputs Into a 50,000 bbl/Day
Shale Oil Plant (1970 dollars)

Electric power	$ 9,300,000
Payments to state and federal government	9,500,000
Wages and salaries	15,000,000
Imports (out of state)	165,200,000
Depreciation	20,000,000
Water	7,200 acre-feet
Water use (consumptive)	32.87 acre feet/10^6 output

In retrospect, other "guesstimates" of additional inputs could have been attempted and probably some of the "imports" (e.g. ceramic balls for retorting) should have been allocated to Colorado. In sum, the economic impacts are biased downward by omitting other positive inputs, but the amount of this bias is difficult to estimate.

Coal mining was characterized as new underground or new strip. For the former, data were obtained from industry sources and a promise of confidentality was made. However, the following classes of inputs were included: wages and benefits, chemicals and explorsives, fuel and power, supplies, and other. In the case of chemicals and explosives, it was assumed that they were available within the State, but not in the UMS or Green Basins. Consumptive water use was estimated to be 6.8 acre-feet per million dollars of output (at $7/ton).

The new strip mining sector was estimated from U.S. Bureau of Mines data, Circular 1972 IC 8535. Estimates were based on a 5 million ton per year operation and are given in Table 4.

Table 4.
Major Inputs Into a 5 Million Ton/Year
Western Strip Mining Operation

Wages and salaries	$850,800
Local taxes	250,000
Federal taxes	314,400
Chemicals & explosives	850,600
Oil and gas	111,000
Electric power	126,000
Water use (consumptive)	326.8 acre-feet/$\$10^6$ output

The same assumption was made regarding the source of the "chemicals and explosives" input. In all cases, strip coal was valued at $2/ton and underground coal, being of much higher quality and heat content suited primarily for metalurgical uses, at $7/ton.

Water

Water "use" must be specified both in terms of how much is withdrawn from the source and how much is actually consumed. Return flows - the difference between withdrawals and consumptive use - can represent a large part of the water diverted (1/2 to 2/3 for residential uses, as much as 1/2 for irrigation) and are quite important to the maintenance of flows for downstream users. It is also necessary to distinguish between direct and indirect water uses.

Water quality in this study is defined as total dissolved solids (TDS), either in tons of total salt load or in concentration. TDS is affected by natural sources, the contents of return flows, and the concentrating effects of consumptive water uses. A change in economic activity will induce both direct and indirect salt loadings and both are computed by the hydro-salinity model.

It is not yet known whether or not serious salt problems will follow from shale oil development. Problems might relate to the use or disposal of brines recovered with the shale and the possible leaching of salts from the spent shale. Industry sources have asserted that these will not be significant sources of pollution. The calculations in this study cover only TDS additions from sanitary and clean-up water uses typical of industry.

Air Pollution

The impacts of the three energy development scenarios include possible degradation of air quality in Rio Blanco, Routt, Moffat, Garfield, Gunnison, and Delta counties. An attempt was made to calculate the dispersion or diffusion of airborne pollutants through the region by use of a mathematical simulation model. In this section, only the direct air pollution impacts of energy growth are considered. Although the input-output framework provides a mechanism by which both direct and indirect effects can be calculated, the scope of this section includes only direct air quality impacts.

All energy extraction scenarios considered here are centered in Northwestern Colorado. This area is typified by a proliferation of ridges, valleys and mesas and is generally quite variable in form and contour. This type of conformation results in local micro-climates influenced less by synoptic (mesoscale) climatic events and more by local (microscale) characteristics. As a result, dispersion of airborne pollutants varies from site to site and can only be modeled approximately by the best of air pollution models now extant.

Mean temperatures for a year range from 40°-60°F and insolation is about 1500 Btu/(ft^2)(day) on a horizontal surface. Precipitation averages from 8 to 16 inches per year in the region. In this arid, sunny coimate, fugitive dust emissions require more control effort than in other areas of the United States. High surface winds associated with the passages of cold fronts may exacerbate the fugitive dust problem at mine sites and temporarily unvegetated areas.

With the exception of the aerological environment of large municipalities, air quality in the region is excellent. However, few data on air quality exist for the area other than measurements of particulate concentrations made near the towns of Meeker, Grand Valley, Rio Blanco and Rangely by the Colorado Department of Health. There are indications that natural particulate hazes from windblown dust may exceed acceptable air quality standards periodically at the present time with no industrial development in the region. Airborne hydrocarbons may exist in some areas of the region resulting from emissions from vegetation (sagebrush).

An air pollutant dispersion model APGDM has been developed at the University of Colorado's Bureau of Economic Research. The model is of the Gaussian type and is described in Udis, et al[4]. This simulation model includes the effects of the following primary variables upon the diffusion of pollutants from a given source into the atmosphere: (1) stack height, exit temperature, exit velocity and plume rise; (2) wind speed, wind direction, ambient temperature, atmospheric stability, temperature gradient, and insolation; (3) inversion depth; (4) background air quality; (5) arbitrary receptor location; (6) terrain variations downwind; (7) arbitrary time period.

Since the behavior of plumes in the present impact areas may not conform to all Gaussian model assumptions, the dispersion results presented in the shale oil impact analysis must be viewed as approximate.

Direct airborne emissions from underground coal mining are negligible. The transportation, storage and distribution phases of underground-mined coal are also very clean since conveyors or trains are used for transport. Surface mining of coal can result in significant air pollution from the mining and transport phases.

Unlike the two coal extraction scenarios considered in this report, the development of the postulated 280,000 bbl/day shale oil extraction industry will have major impacts on the air quality in Rio Blanco and Garfield Counties. Since sufficient technical data were available only on the TOSCO II process, it has been assumed that all plants are to use that process so that the related calculation can be demonstrated. Estimates of emissions from a steady state TOSCO II plant with underground shale mining have been based on the Environmental Impact Statement prepared by the Colony Development Operation[12] for their proposed 50,000 bbl/day facility to be located at Parachute Creek, Colorado. Significant emissions arise from some 17 phases of the operation including shale transport and crushing, retorting, power plant operation, and on-site kerogen storage. Cementation reactions and revegetation are assumed to control fugitive dust from large spent shale disposal areas. The total annual emissions from one 50,000 bbl/day TOSCO II plant and from the seven plants postulated in the present scenario are shown in Table 5.

The calculated emissions agree with those presented in the FEA Project Independence Oil Shale Task Force Report[13] with the exception of NO_X emissions. The FEA report, inexplicably, does not include the dominant NO_X emitter of the TOSCO II process (raw shale preheat system). Fugitive dust emissions are expected to be much smaller (46TPY for 50000 B/D plant) than those associated with the procession plant[13].

Table 5
Annual Direct Emissions From Shale Oil Extraction (tons/year)* Assuming TOSCO II Technology

Pollutant	Production Level 50,000 B/D	 280,000 B/D
Particulates	3075	17220
SO_2	6950	38920
NO_X	24600	137760
CO	250	1400
Hydrocarbons	1700	9520

---

* These figures are based on the assumption that all shale oil projects would be using the TOSCO II process and experiencing a 90% load factor at each plant.

Model outputs are in terms of incremental pollution increases for the region surrounding each of the seven postulated plants considered. The physical distributions of long term average pollution are presented on isopleth (constant pollutant quantity) maps which are a convenient visual means of determining the nature of pollutant distribution in the areas around a given source. Incremental isopleth maps for SO_2 and NO_X are illustrated in Figure 1.

Results

Selected results are given in Tables 6-11 below.

Table 6
Total Output Impacts of Energy Developments
(millions of 1970 dollars)

	Shale Oil	UG Coal	Strip Coal	Total
UMS Basin	722	120	-	842
Green Basin	800	-	33	833
Statewide	1,654	171	47	1,872
% 1970	4.3%	0.4%	0.1%	4.9%

Table 7
Total Increases in Income Payments to Colorado Households
(millions of 1970 dollars)

	Shale Oil	UG Coal	Strip Coal	Total
UMS Basin	64	24	-	88
Green Basin	72	-	3.9	76
Statewide	136	27	3.9	167
% 1970	1.7%	0.3%	0.05%	2.1%

Table 8
Total Increases in Employment

	Shale Oil	UG Coal	Strip Coal	Total
UMS Basin	6,480	4,326	-	10,806
Green Basin	7,525	-	1,206	8,731
Statewide	16,670	4,964	1,300	22,934
% 1970	2.0%	0.6%	0.2%	2.7%

Table 9
UMS Increases in Annual Consumptive Use and Salt Loadings

	Shale Oil	New UG Coal	Both
Increased consumptive use (AF/yr)	31,320	348	31,668
Increased salt loading (ton/yr)	3,444	132	3,576

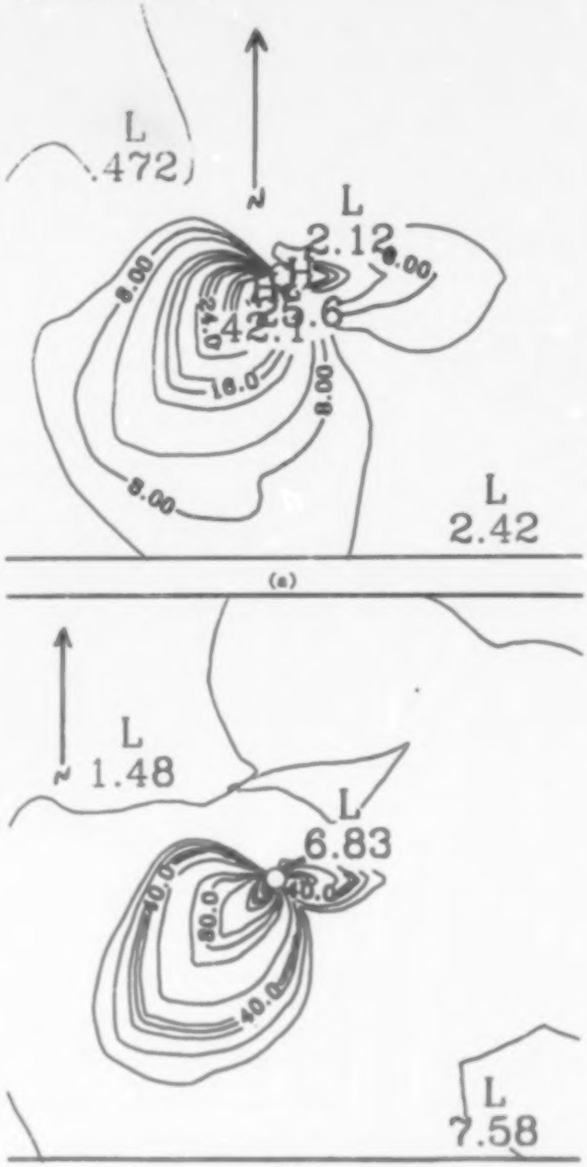
Table 10
White River Increases in Annual Consumptive Use and Salt Loadings

	Shale Oil
Increased consumptive use (AF/yr)	34,164
Increased salt loading (tons/yr)	5,568

Table 11
Yampa River Increases in Annual Consumptive Use and Salt Loadings

	New Strip Coal	Coal & Spillovers*
Increased consumptive use (AF/yr)	8,148	8,520
Increased salt loading (tons/yr)	2,172	3,204

*Economic spillovers from shale oil development in White River Basin.



(a)

(b)

Figure 1. Longterm Average Isopleth Maps for Rio Blanco (c-a Tract) (50,000 bbl/day) for SO_2 and NO_x; 250,000 series map, contour intervals 2 and 10 mcg/cubic meter, respectively.

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CSMP CONCEPT AND APPLICATIONS TO ENVIRONMENTAL MODELING AND SIMULATION

Grace Chang and C. Lindsay Wang
Systems Architects, Inc.
Arlington, Virginia

ABSTRACT

The Continuous System Modeling Program (CSMP) is a continuous system simulation language that allows models to be prepared directly and simply from either a block diagram representation or a set of differential equations. A CSMP program is constructed from three types of statements: Structure Statements which define the model, Data Statements which assign numerical values to parameters, constraints and initial conditions, and Control Statements which specify the execution and report generation options. CSMP accepts most FORTRAN statements to supply the user with logic and algebraic capability. Computer graphics and interactive execution capabilities are also available in CSMP.

In this paper, the fundamental concepts of CSMP that are related to environmental modeling and simulation are summarized. Procedures for applying the concept to environmental models are described. Sample cases for environmental problems are presented.

CSMP OVERVIEW

Continuous System Modeling Program III (CSMP III) is an IBM program product which aids development and execution of simulation models for continuously changing systems. It is written in FORTRAN IV language and ASSEMBLER language, and has been installed at many IBM 360/370 facilities.

CSMP III is a continuous system simulation language (CSSL) that allows the digital simulation of continuous processes on large-scale digital machine.

The program provides an application-oriented language which permits models to be prepared directly and simply from either a block diagram representation or a set of ordinary differential equations. It includes a basic set of functional blocks (also called functions) which can represent the components of a continuous system and accepts application-oriented statements defining the connections between these functional blocks.

A CSMP III program is constructed from three types of statements:

Structure Statements - which define the model. They consist of FORTRAN statements and functions, and functional blocks (also called functions) designed for CSMP.

Data Statements - which assign numerical values to parameters, constants and initial conditions.

Control Statements - which specify options for the execution of the program and the choice of output.

It accepts FORTRAN statements, thus supplying the user with logical and algebraic capability. Hence the user can readily handle complex nonlinear and time-variant problems.

This program is specifically designed to satisfy the needs of scientists and engineers, who wish to simulate physical phenomenon without having to spend time and resources learning the intricacies of sophisticated computer programming.

Applications in which CSMP III can be used include studies of nuclear reactors, control system design, parameter estimation, studies of blood circulation and other physiological processes, studies of chemical refineries, natural gas transmission, process control, investigation of aircraft landing and take-off, plant growth, natural resources management, simulation of corporate financial policies and industrial dynamics.

CSMP III has the following basic functional capabilities:

- Powerful Standard Functions - The CSMP III language contains 42 powerful simulation functions for performing such operations as integration, differentiation, signal and function generation, Laplace transformation, switching and logical operations.
- Capability to Develop Additional Functions - By combining standard CSMP III functions and/or FORTRAN statements, the user may build larger, more powerful functions specifically suited to his particular field of study. These functions become part of his CSMP III language and they may be used in a manner identical to the

standard CSMP III functions.

- Extensive Function Generation Capability - The user may incorporate arbitrary or experimental data into his model. Such data may be the function of one or two variables. Interpolation between data points is handled automatically, including interpolation of functions of two variables.

- Powerful Array-Handling Capability - The storage, manipulation, and printing of arrays is easily performed. Integrator arrays are also easily specified and handled.

- FORTRAN-Based System - FORTRAN statements can be intermixed (with a few minor exceptions) with CSMP III statements, thereby placing the logic and algebraic capability of the FORTRAN language at the user's disposal.

- Extensive Library Facilities - The library facilities of CSMP III allow the user to develop and maintain libraries of functions, sub-models, arbitrary or experimental data, tables, and complete models.

- Wide Selection of Integration Algorithms - The user has a wide range of integration algorithms from which to choose - both single and double precision; fixed and variable step, including one specifically designed for "stiff" equations.

- Numerous Output Options - The values of one through 55 selected variables may be printed during the simulation run.

- Improved Coding and Debugging Aids - The CSMP III language - including FORTRAN when used in conjunction with CSMP III - is free-form. Extensive debugging aids are available to the user to check out his CSMP III and his FORTRAN coding.

- Flexible Installation - CSMP III may be tailored to the user's particular hardware configuation.

The CSMP III graphic feature provides the following capabilities:

- Interactive Interrogation of Results - Using the graphic device (such as IBM 2250 graphic display terminal), the user may quickly display and analyze the results of the simulation run and select those variables which are to be printed or print-plotted for later reference and evaluation.

  One to four grids may be simultaneously displayed, with one to four variables plotted per grid.

  Graphic plots to logarithmic scales are readily available.

  The value of a plotted variable may be obtained merely by touching the display with the light pen at the appropriate point on the curve.

- On-Line Reference Manual - Whenever the user is in doubt about the user of a CSMP III statement, he can immediately obtain a graphical display of instructional messages relating to rules and proper usage.

- Interactive Simulation Run Control - By dynamically displaying selected variables during a simulation run, the user can monitor the simulation and interrupt the run at will to change the model, model data, execution specifications or to vary the display itself.

- Interactive Model Development - With its highly versatile set of editing features, Graphic CSMP III makes it easy for the user to develop simulation models, completely "on-line".

  With merely a few touches of the light pen, the user may store and retrieve data, sub-models, or entire models using the CSMP III library. This assures continuity of model development and helps the individual user to quickly incorporate commonly used sub-models and data into his model.

CSMP OPERATION OVERVIEW

CSMP III uses five phases, in the following order to build and execute a CSMP III model: Input Processor, Translator, FORTRAN, Linkage Editor, and Execution.

1. The Input Processor phase reads the next CSMP III model from the Input file, accesses and retrieves any data referenced in the symbolic library by INCLUDE statements, and builds the input for the Translator phase.

2. The Translator phase analyzes the CSMP III statements from the Translator input file and builds two separate files: a FORTRAN input file containing FORTRAN subprograms representing the logic of the CSMP III model's structure, and an Execution input file containing the CSMP III data and execution control statements.

3. The FORTRAN phase converts the FORTRAN subprograms from the Translator phase to a machine-language object module.

4. The Linkage Editor phase combines the machine-language object module produced by the FORTRAN phase with the precompiled CSMP III load module library (for integration, plotting, etc.) to produce the Execution phase load module.

5. The Execution phase (built by the Linkage Editor phase) first interprets the data and execution control statements from the Translator phase for the next run and then proceeds to execute that simulation run, storing simulation results on the Prepare

data set when required. This is repeated until all the execution runs have been exhausted. Print documents are generated during each execution run, while output documents are generated at the end of each execution case.

STRUCTURE OF THE MODEL

The CSMP formulation of a model is divided into three segments - INITIAL, DYNAMIC and TERMINAL - that describe, respectively, the computations to be performed before, during and after each solution.

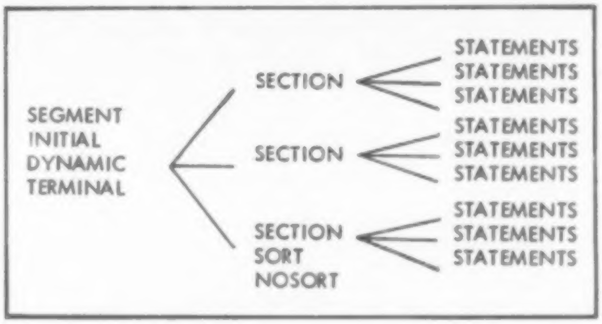
INITIAL Segment - which is intended exclusively for the computation of initial condition values and those parameters that the user prefers to express in terms of the more basic parameters. This segment is optional.

DYNAMIC Segment - which is the most extensive in the model. It contains the complete description of the systems dynamics, together with any other computations required during the solution of the system. The structure statements within this segment are generally a mixture of CSMP and FORTRAN statements.

The DYNAMIC segment is required. This segment may be declared explicitly by a DYNAMIC statement or implicitly by the absence of INITIAL, DYNAMIC, or TERMINAL statements.

TERMINAL Segment - which is used for these computations required at the end of the run, after completion of the solution. This segment is optional.

These segments represent the highest level of the structure hierarchy. Each of the segments may include one or more sections which represent rational groupings of the structure statements and may be processed as either paralleled or procedural entities.



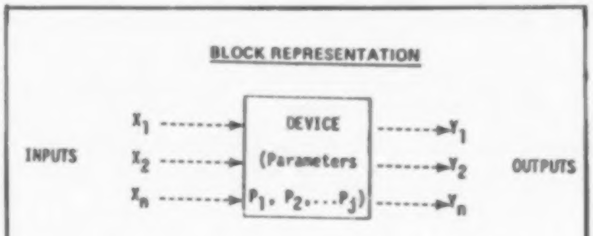
Structure of the CSMP IV Model

These sections contain the structure statements that specify model dynamics and associated computations.

ELEMENTS OF THE CSMP III

The basic elements in the preparation of CSMP statements are:

1. NUMERICAL CONSTANTS - which are unchanging quantities specified in numeric form in the input statements.
2. SYMBOLIC NAMES - which represent quantities that may either change during a run or be changed by the program between successive runs of the same model structure.
3. OPERATORS - which are used instead of functional blocks to indicate basic arithematical functions or relationships. As in FORTRAN, these operators are +, -, *, /, **, + and ( ).
4. FUNCTIONAL BLOCKS - which are used for more complex mathematical operations, such as: integration, time delay, quantization and limiting.



MATHEMATICAL EXPRESSION

$$Y_1, Y_2, \ldots, Y_n = f(P_1, P_2, \ldots P_j, X_1, X_2 \ldots X_n)$$

EQUIVALENT CSMP III STATEMENT

```
Y1,Y2,....YM=DEVICE(P1,P2,...P5,X1,X2,....XN)
```

Example:

```
Y = INTERL(IC,X)
```

which states the output, Y, is obtained by integrating X, with Y at the starting time is equal to IC.

5. LABELS - which are the first word of CSMP data and control statements that tell the program the purpose of the statement. Some

statements contain only the label, such as INITIAL, NOSORT, and NEDMAC. Other contain a label and appropriate data.

Example:

```
TIMER          DELT = 0.025          FINTIM = 100
```

which specifies the integration interval and the "finish time" for a run.

PROBLEM DESCRIPTION

Oxygen balance studies of a polluted stream usually result in one or more dissolved oxygen profiles along the course of the stream. Dissolved oxygen is a very commonly used water quality criterion; it is an important general index of quality albeit not all-pervasive.

Following is a general equation describing dissolved oxygen relations in a stream receiving oxygen-consuming waste:

$$\frac{dB}{dt} = -(K_1 + K_3)B + R \; . \; . \; . \; . \; . \quad (1)$$

where

$\frac{dB}{dt}$ = The rate of change of BOD (Biochemical Oxygen Demand) with respect to time

B = BOD present

R = The rate of BOD addition due to runoff and scour

K_1 = The rate constant for deoxygenation

K_3 = The rate constant for sedimentation

A related expression, using dissolved oxygen deficit, D, rather than BOD, B is the rollowing:

$$\frac{dD}{dt} = K_1 B - K_2 D - A \; . \; . \; . \; . \; . \quad (2)$$

where

$\frac{dD}{dt}$ = The rate of change of dissolved oxygen deficit with respect to time

D = The existing oxygen deficit (the difference between the saturation concentration and the existing dissolved oxygen concentration)

A = The net rate of oxygen production due to photosynthesis and respiration of phytoplanton and/or waterweeds

K_2 = The rate constant for reaeration

Integrating these two equations, we get:

$$B_t = (B_o - \frac{R}{K_1 + K_3})e^{-(K_1 + K_3)t} + \frac{R}{K_1 + K_3} \qquad (3)$$

and

$$D_t = \frac{K_1}{K_2 - K_1 - K_3}(B_o - \frac{R}{K_1 + K_3})(e^{-(K_1 + K_3)t} - e^{-K_2 t})$$

$$+ \frac{K_1}{K_2}(\frac{R}{K_1 + K_3} - \frac{A-}{K_1})(1 - e^{-K_2 t}) + D_o e^{-K_2 t} \quad (4)$$

Equation (4) describes the typical oxygen sag curve as illustrated in Figure 1. To the left of tc in the figure, deoxygenation exceeds reaeration, to the right of tc, the reverse is the case. The so-called critical time, tc, is the moment at which dissolved oxygen reaches its lowest value. From stream flow information (velocity), the location of the critical point in the river course can be determined.

Here, suppose that a solution is to be obtained from:

K_1 = 0.26 and 0.27 $(day)^{-1}$

K_2 = 0.11 $(day)^{-1}$

K_3 = 0.36 $(day)^{-1}$

A = 0.43 ppm/day (ppm = parts per million)

R = 2.8 ppm/day

D_o = 5.2 ppm

B_o = 6.9 ppm

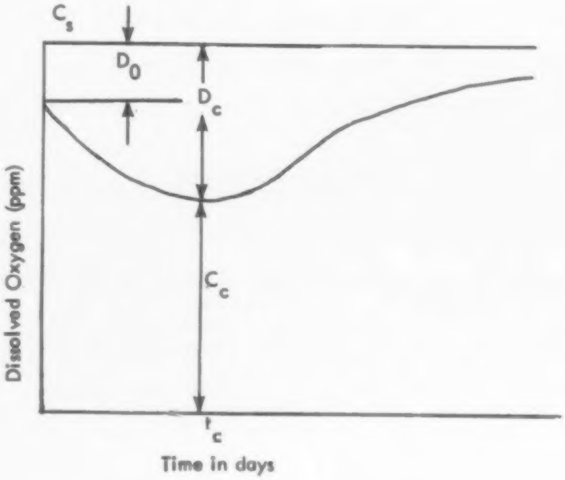


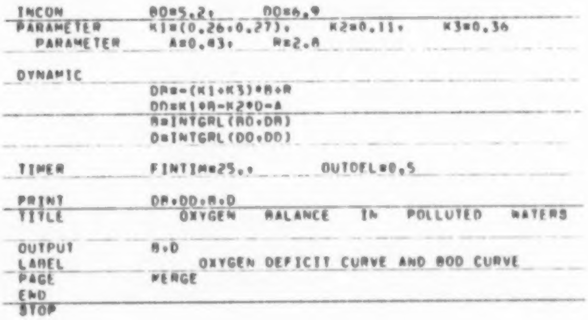
FIGURE 1 OXYGEN SAG CURVE

On the oxygen sag curve. C_s is dissolved oxgen (DO) saturation; D_o is initial DO deficit; D_c is critical DO deficit; C_c is critical DO level

MODEL DESCRIPTION

Figure 2 shows a complete listing of the CSMP III statements for the sample problem.

The INCON and PARAMETER statements assign the values of initial conditions and parameters. K_1 = (0.26, 0.27) means that two simulation runs will be made; each with a different K_1 value. DYNAMIC card indicates the end of the initialization statements, and the beginning of the dynamic portion of the simulation. The INTGRL function is used to perform integration. TIMER FINTIM specifies the finish time for terminating this simulation. OUTDEL indicates the time interval of output printing and plotting. PRINT statement presents the variables which are printed during execution of the run. TITLE allows the user to specify the text of a heading to appear at the top of each page of the print document. OUTPUT statement lists the variables to be print-plotted after completion of the case. LABEL specifies the text of a heading appearing at the top of each page of the print-plot document. PAGE MERGE indicates that two curves, B and D, are to be merged on a single output print-plot. The END and STOP statements define the end of the model.



```
INCON          BO=5.2,     DO=6.9
PARAMETER      K1=(0.26,0.27),     K2=0.11,     K3=0.36
  PARAMETER     A=0.43,     R=2.8

DYNAMIC
               DB=-(K1+K3)*B+R
               DD=K1*B-K2*D-A
               B=INTGRL(BO,DB)
               D=INTGRL(DO,DD)

TIMER          FINTIM=25.,          OUTDEL=0.5

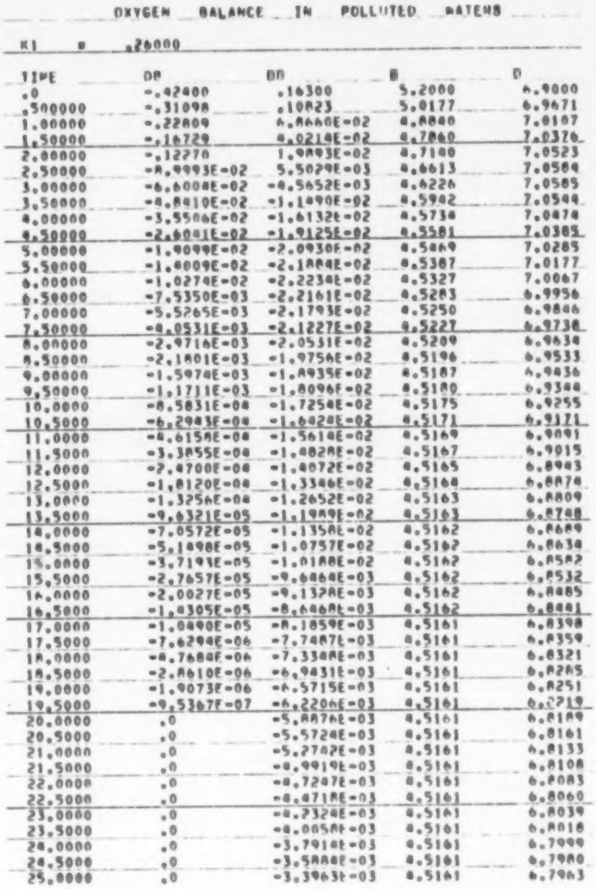
PRINT          DB,DD,B,D
TITLE             OXYGEN   BALANCE   IN   POLLUTED   WATERS

OUTPUT         B,D
LABEL              OXYGEN DEFICIT CURVE AND BOD CURVE
PAGE           MERGE
END
STOP
```

FIGURE 2 SAMPLE INPUT

RESULT

Figures 3, 4, 5 and 6 show the tabular printing output and merged print-plotting output for the run with a K_1 = 0.26 and 0.27 respectively. From these outputs we can find the critical time is 3.0 and critical oxygen deficit is 7.0585 for K_1 = 0.26, and the critical time is 4, critical oxygen deficit is 7.1567 for K_1 = 0.27, respectively.



```
              OXYGEN   BALANCE   IN   POLLUTED   WATERS

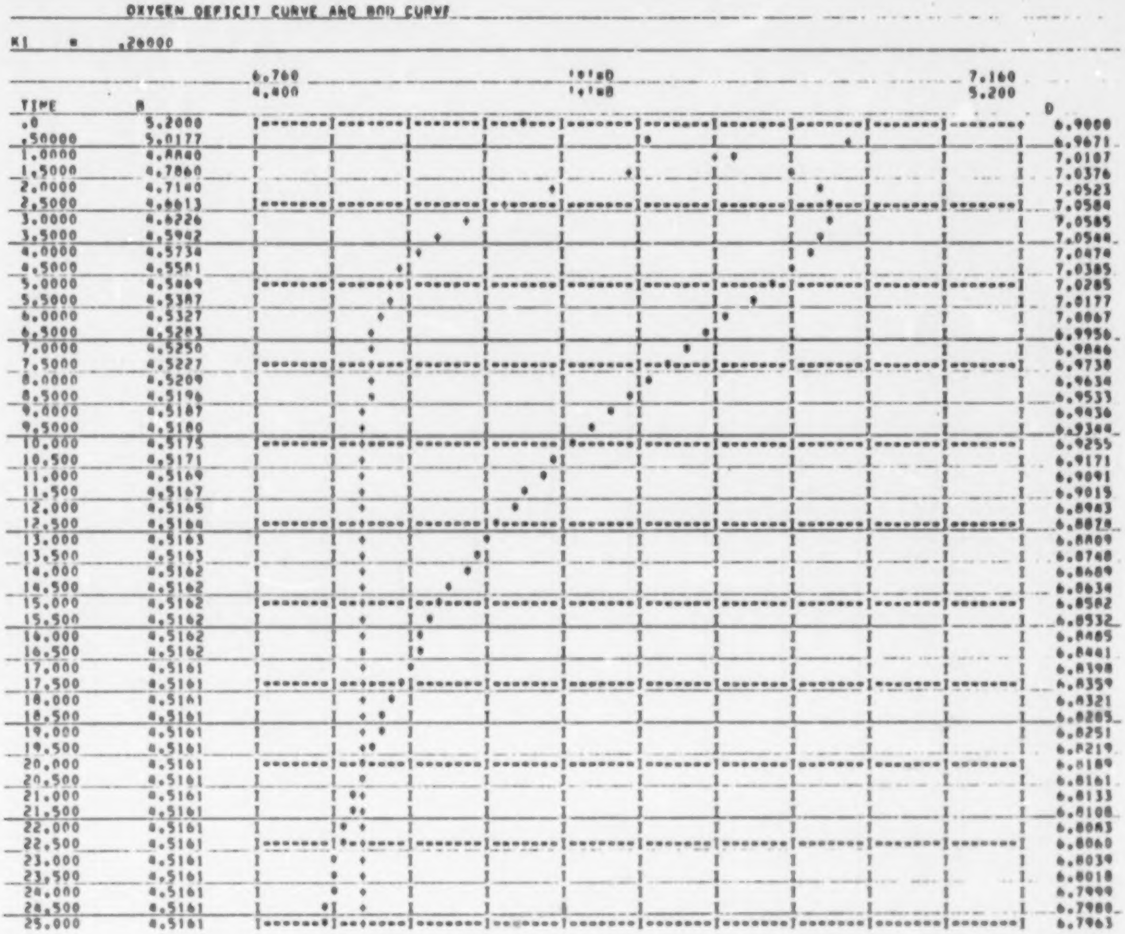
 K1     =     .26000

 TIME           DB              DD              B               D
 .0             -.42400          .16300         5.2000          6.9000
 .500000        -.31098          .10823         5.0177          6.9671
 1.00000        -.22809         6.8660E-02      4.8840          7.0107
 1.50000        -.16729         4.0214E-02      4.7860          7.0376
 2.00000        -.12270         1.9893E-02      4.7100          7.0523
 2.50000        -8.9993E-02     5.5029E-03      4.6613          7.0584
 3.00000        -6.6004E-02    -4.5652E-03      4.6226          7.0585
 3.50000        -4.8410E-02    -1.1490E-02      4.5942          7.0544
 4.00000        -3.5506E-02    -1.6132E-02      4.5734          7.0474
 4.50000        -2.6041E-02    -1.9125E-02      4.5581          7.0385
 5.00000        -1.9099E-02    -2.0930E-02      4.5469          7.0285
 5.50000        -1.4009E-02    -2.1884E-02      4.5387          7.0177
 6.00000        -1.0274E-02    -2.2234E-02      4.5327          7.0067
 6.50000        -7.5350E-03    -2.2161E-02      4.5283          6.9956
 7.00000        -5.5265E-03    -2.1793E-02      4.5250          6.9846
 7.50000        -4.0531E-03    -2.1227E-02      4.5227          6.9738
 8.00000        -2.9716E-03    -2.0531E-02      4.5209          6.9634
 8.50000        -2.1801E-03    -1.9756E-02      4.5196          6.9533
 9.00000        -1.5974E-03    -1.8935E-02      4.5187          6.9436
 9.50000        -1.1711E-03    -1.8096E-02      4.5180          6.9344
 10.0000        -8.5831E-04    -1.7254E-02      4.5175          6.9255
 10.5000        -6.2943E-04    -1.6428E-02      4.5171          6.9171
 11.0000        -4.6158E-04    -1.5614E-02      4.5169          6.9091
 11.5000        -3.3855E-04    -1.4828E-02      4.5167          6.9015
 12.0000        -2.4700E-04    -1.4072E-02      4.5165          6.8943
 12.5000        -1.8120E-04    -1.3346E-02      4.5164          6.8874
 13.0000        -1.3256E-04    -1.2652E-02      4.5163          6.8809
 13.5000        -9.6321E-05    -1.1989E-02      4.5163          6.8748
 14.0000        -7.0572E-05    -1.1358E-02      4.5162          6.8689
 14.5000        -5.1498E-05    -1.0757E-02      4.5162          6.8634
 15.0000        -3.7193E-05    -1.0188E-02      4.5162          6.8582
 15.5000        -2.7657E-05    -9.6464E-03      4.5162          6.8532
 16.0000        -2.0027E-05    -9.1328E-03      4.5162          6.8485
 16.5000        -1.4305E-05    -8.6468E-03      4.5162          6.8441
 17.0000        -1.0490E-05    -8.1859E-03      4.5161          6.8398
 17.5000        -7.6294E-06    -7.7487E-03      4.5161          6.8359
 18.0000        -4.7684E-06    -7.3348E-03      4.5161          6.8321
 18.5000        -2.8610E-06    -6.9431E-03      4.5161          6.8285
 19.0000        -1.9073E-06    -6.5715E-03      4.5161          6.8251
 19.5000        -9.5367E-07    -6.2206E-03      4.5161          6.8219
 20.0000         .0            -5.8876E-03      4.5161          6.8189
 20.5000         .0            -5.5724E-03      4.5161          6.8161
 21.0000         .0            -5.2742E-03      4.5161          6.8133
 21.5000         .0            -4.9919E-03      4.5161          6.8108
 22.0000         .0            -4.7247E-03      4.5161          6.8083
 22.5000         .0            -4.4718E-03      4.5161          6.8060
 23.0000         .0            -4.2324E-03      4.5161          6.8039
 23.5000         .0            -4.0058E-03      4.5161          6.8018
 24.0000         .0            -3.7914E-03      4.5161          6.7999
 24.5000         .0            -3.5884E-03      4.5161          6.7980
 25.0000         .0            -3.3963E-03      4.5161          6.7963
```

FIGURE 3 TABULAR PRINTING OUTPUT (K_1 = 0.26)

REFERENCES

1. CSMP III Program Reference Manual (SH19-7001-2) IBM Corporation (1972)
2. CSMP III and Graphic Feature General Information (GH19-7000-1), IBM Corporation (1971)
3. CSMP III Operations Guide (SH19-7002-1), IBM Corporation (1972)
4. CSMP III Graphic Feature Program Reference Manual (SH19-7003-1), IBM Corporation (1972)
5. CSMP III Graphic Feature Operations Guide (SH19-7004-1) IBM Corporation (1972)
6. Gordon, Geoffrey, "System Simulation," Prentice-Hall, Inc. (1969)
7. Leonard, Caiccio, Water and Water Pollution Handbook, Volume 1, Marcel Dekker, Inc., New York (1971)
8. Thomas R. Camp, Water and Its Impurities, Reinhold Publishing Corporation, (1963)



```
              OXYGEN DEFICIT CURVE AND BOD CURVE
K1     =     .26000

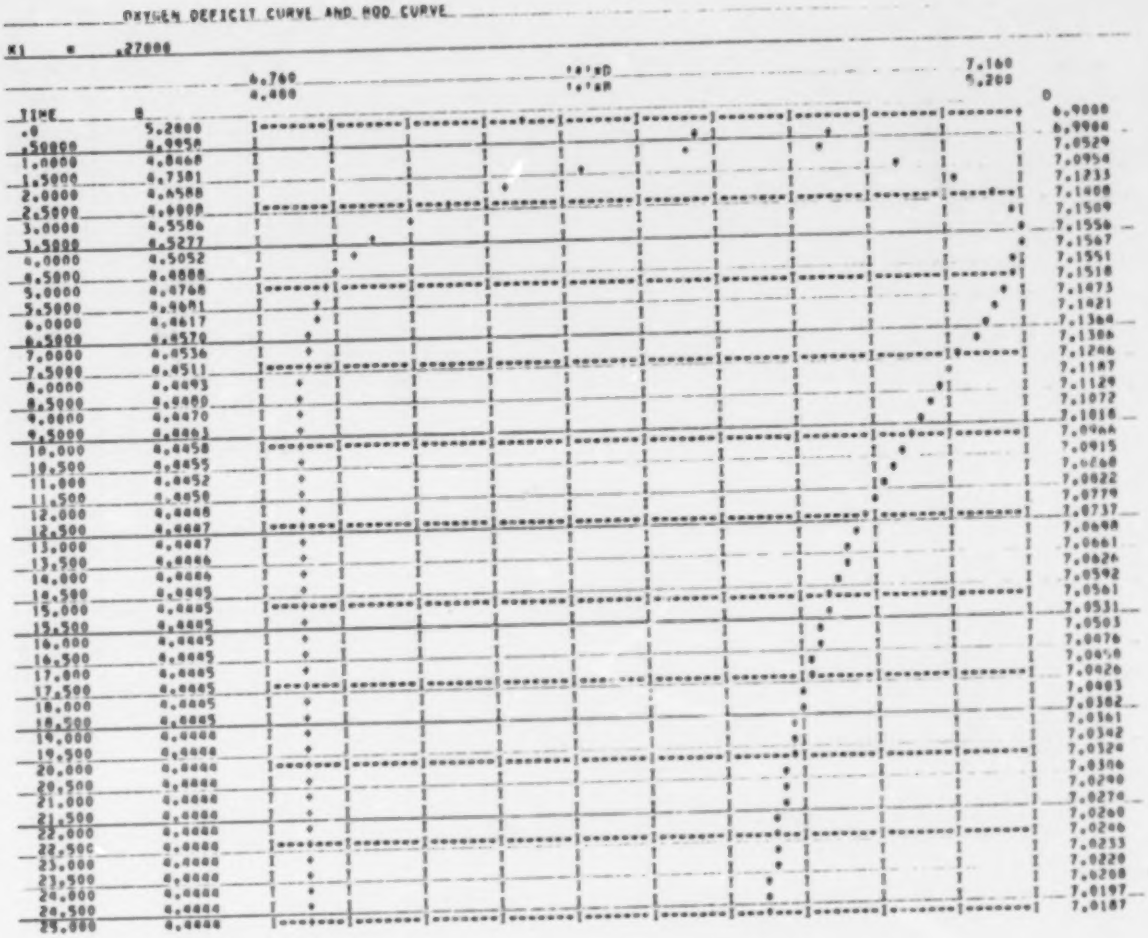
TIME           B                D
.0             5.2000           6.9000
.50000         5.0177           6.9671
1.0000         4.8840           7.0107
1.5000         4.7860           7.0376
2.0000         4.7140           7.0523
2.5000         4.6613           7.0584
3.0000         4.6226           7.0585
3.5000         4.5942           7.0544
4.0000         4.5734           7.0474
4.5000         4.5581           7.0385
5.0000         4.5469           7.0285
5.5000         4.5387           7.0177
6.0000         4.5327           7.0067
6.5000         4.5283           6.9956
7.0000         4.5250           6.9846
7.5000         4.5227           6.9738
8.0000         4.5209           6.9634
8.5000         4.5196           6.9533
9.0000         4.5187           6.9436
9.5000         4.5180           6.9344
10.000         4.5175           6.9255
10.500         4.5171           6.9171
11.000         4.5169           6.9091
11.500         4.5167           6.9015
12.000         4.5165           6.8943
12.500         4.5164           6.8874
13.000         4.5163           6.8809
13.500         4.5163           6.8748
14.000         4.5162           6.8689
14.500         4.5162           6.8634
15.000         4.5162           6.8582
15.500         4.5162           6.8532
16.000         4.5162           6.8485
16.500         4.5162           6.8441
17.000         4.5161           6.8398
17.500         4.5161           6.8359
18.000         4.5161           6.8321
18.500         4.5161           6.8285
19.000         4.5161           6.8251
19.500         4.5161           6.8219
20.000         4.5161           6.8189
20.500         4.5161           6.8161
21.000         4.5161           6.8133
21.500         4.5161           6.8108
22.000         4.5161           6.8083
22.500         4.5161           6.8060
23.000         4.5161           6.8039
23.500         4.5161           6.8018
24.000         4.5161           6.7999
24.500         4.5161           6.7980
25.000         4.5161           6.7963
```

FIGURE - 4 PRINT-PLOTTING (k1= 0.26)

```
            OXYGEN   BALANCE   IN   POLLUTED   WATERS
K1     =     .27000

TIME        DB             DD             B           D
.0          -.47600        .21500         5.2000      6.9000
.500000     -.30738        .14994         4.9958      6.9904
1.00000     -.25351        .10283         4.8868      7.0529
1.50000     -.18501        6.8801E-02     4.7381      7.0954
2.00000     -.13502        4.4303E-02     4.6588      7.1233
2.50000     -9.8535E-02    2.6740E-02     4.6008      7.1408
3.00000     -7.1909E-02    1.4222E-02     4.5586      7.1509
3.50000     -5.2478E-02    5.3702E-03     4.5277      7.1556
4.00000     -3.8298E-02    -8.2225E-04    4.5052      7.1567
4.50000     -2.7948E-02    -5.0868E-03    4.4888      7.1551
5.00000     -2.0396E-02    -7.9593E-03    4.4768      7.1518
5.50000     -1.4885E-02    -9.8285E-03    4.4681      7.1473
6.00000     -1.0862E-02    -1.0978E-02    4.4617      7.1421
6.50000     -7.9269E-03    -1.1612E-02    4.4570      7.1364
7.00000     -5.7840E-03    -1.1883E-02    4.4536      7.1306
7.50000     -4.2210E-03    -1.1898E-02    4.4511      7.1246
8.00000     -3.0794E-03    -1.1736E-02    4.4493      7.1187
8.50000     -2.2478E-03    -1.1454E-02    4.4480      7.1129
9.00000     -1.6394E-03    -1.1094E-02    4.4470      7.1072
9.50000     -1.1959E-03    -1.0685E-02    4.4463      7.1018
10.0000     -8.7261E-04    -1.0248E-02    4.4458      7.0966
10.5000     -6.3705E-04    -9.7980E-03    4.4455      7.0915
11.0000     -4.6444E-04    -9.3449E-03    4.4452      7.0868
11.5000     -3.3855E-04    -8.8975E-03    4.4450      7.0822
12.0000     -2.4700E-04    -8.4593E-03    4.4448      7.0779
12.5000     -1.7929E-04    -8.0343E-03    4.4447      7.0737
13.0000     -1.3065E-04    -7.6247E-03    4.4447      7.0698
13.5000     -9.5367E-05    -7.2313E-03    4.4446      7.0661
14.0000     -6.8665E-05    -6.8554E-03    4.4446      7.0626
14.5000     -4.9591E-05    -6.4967E-03    4.4445      7.0592
15.0000     -3.5286E-05    -6.1544E-03    4.4445      7.0561
15.5000     -2.5749E-05    -5.8296E-03    4.4445      7.0531
16.0000     -1.8120E-05    -5.5203E-03    4.4445      7.0503
16.5000     -1.2398E-05    -5.2267E-03    4.4445      7.0476
17.0000     -8.5831E-06    -4.9487E-03    4.4445      7.0450
17.5000     -5.7220E-06    -4.6846E-03    4.4445      7.0426
18.0000     -3.8147E-06    -4.4348E-03    4.4445      7.0403
18.5000     -2.8610E-06    -4.1983E-03    4.4445      7.0382
19.0000     -1.9073E-06    -3.9735E-03    4.4444      7.0361
19.5000     -9.5367E-07    -3.7617E-03    4.4444      7.0342
20.0000     .0             -3.5603E-03    4.4444      7.0324
20.5000     .0             -3.3697E-03    4.4444      7.0306
21.0000     .0             -3.1893E-03    4.4444      7.0290
21.5000     .0             -3.0184E-03    4.4444      7.0274
22.0000     .0             -2.8568E-03    4.4444      7.0260
22.5000     .0             -2.7038E-03    4.4444      7.0246
23.0000     .0             -2.5590E-03    4.4444      7.0233
23.5000     .0             -2.4220E-03    4.4444      7.0220
24.0000     .0             -2.2922E-03    4.4444      7.0208
24.5000     .0             -2.1695E-03    4.4444      7.0197
25.0000     .0             -2.0533E-03    4.4444      7.0187
```

FIGURE - 5 TABULAR PRINTING OUTPUT (K1=0.27)



```
          OXYGEN DEFICIT CURVE AND BOD CURVE

K1    =    .27000

                              6.760                '*'=D                      7.160
                              4.400                '+'=B                      5.200
                                                                                     D
 TIME         B
  .0          5.2000                                                                6.9000
  .50000      4.9950                                                                6.9904
 1.0000       4.8468                                                                7.0529
 1.5000       4.7301                                                                7.0954
 2.0000       4.6588                                                                7.1233
 2.5000       4.6008                                                                7.1408
 3.0000       4.5586                                                                7.1509
 3.5000       4.5277                                                                7.1556
 4.0000       4.5052                                                                7.1567
 4.5000       4.4888                                                                7.1551
 5.0000       4.4768                                                                7.1518
 5.5000       4.4681                                                                7.1473
 6.0000       4.4617                                                                7.1421
 6.5000       4.4570                                                                7.1364
 7.0000       4.4536                                                                7.1306
 7.5000       4.4511                                                                7.1246
 8.0000       4.4493                                                                7.1187
 8.5000       4.4480                                                                7.1129
 9.0000       4.4470                                                                7.1072
 9.5000       4.4463                                                                7.1018
10.000        4.4458                                                                7.0966
10.500        4.4455                                                                7.0915
11.000        4.4452                                                                7.0868
11.500        4.4450                                                                7.0822
12.000        4.4448                                                                7.0779
12.500        4.4447                                                                7.0737
13.000        4.4447                                                                7.0698
13.500        4.4446                                                                7.0661
14.000        4.4446                                                                7.0626
14.500        4.4445                                                                7.0592
15.000        4.4445                                                                7.0561
15.500        4.4445                                                                7.0531
16.000        4.4445                                                                7.0503
16.500        4.4445                                                                7.0476
17.000        4.4445                                                                7.0450
17.500        4.4445                                                                7.0426
18.000        4.4445                                                                7.0403
18.500        4.4445                                                                7.0382
19.000        4.4444                                                                7.0361
19.500        4.4444                                                                7.0342
20.000        4.4444                                                                7.0324
20.500        4.4444                                                                7.0306
21.000        4.4444                                                                7.0290
21.500        4.4444                                                                7.0274
22.000        4.4444                                                                7.0260
22.500        4.4444                                                                7.0246
23.000        4.4444                                                                7.0233
23.500        4.4444                                                                7.0220
24.000        4.4444                                                                7.0208
24.500        4.4444                                                                7.0197
25.000        4.4444                                                                7.0187
```

FIGURE - 6   PRINT-PLOTTING (k1=0.27)

GASP IV CONCEPTS APPLICABLE TO ENVIRONMENTAL MODELING AND SIMULATION

A. Alan B. Pritsker
Purdue University and Pritsker & Associates, Inc.
Lafayette, Indiana

Abstract

Environmental modeling and simulation involves the characterization of a system in order to determine the dynamic performance of the system over a specified period of time. To obtain this dynamic portrayal of the system variables, it is necessary to identify and model the state variables of the system and the points in time at which logical decisions are made to change the status of the system. There has been a growing trend to model systems that involve continuous variables with discrete events superimposed in order to alter the behavior of the system status. This paper presents the fundamental concepts of the GASP IV simulation language that are used to obtain combined simulations. Specifically the paper includes definitions and explanations of the following basic simulation concepts: system status representation; time-events and state-events; time advance procedures; and data collection and analysis. Two examples of combined models are presented that illustrate the concepts as applied to environmental modeling and simulation:

1) Simulation of electroplating operations to evaluate different operating procedures and control policies regarding metal flow and concentration levels; and
2) A model of an urban area with discrete events superimposed.

This paper presents new modeling and simulation concepts that are useful for resolving environmental problems.

Description of GASP IV [8,9,10,17]

GASP IV is a FORTRAN based simulation language that can be used for discrete, continuous, or combined simulation.* The interactions between discretely and continuously changing variables are easily modeled in GASP IV. Extensive use and applications have been made of GASP IV.

In GASP IV a system is modeled in two dimensions, the time dimension and the state-space dimension. These dimensions are further decomposed into manageable elements. In the time dimension this involves the defining of events and the potential changes to the system when an event occurs. The user must specify the causal mechanisms by which events can occur. GASP IV, however, sequences these events in simular time. Thus, the user must define only the mathematical-logical relations that transpire at an event occurrence, and he is not required to model the timing of the events during the simulation.

In the state-space dimension the system is decomposed into its entities which are described by attributes. The attributes are further classified as discrete or continuous. The value of a discrete attribute remains constant between event times. The value of a continuous attribute, hereafter referred to as a state variable, may change between event times according to a prescribed dynamic behavior. Special storage arrays are provided by GASP IV for storing values of state variables and, if required, their derivatives and immediate past values.

A dynamic simulation is then obtained by modeling the events of the system and by advancing time from one event to the next. Events usually cause changes in the status of the system or in the equations defining the state variables of the system. However, change, either discrete or continuous, need not occur at an event time. Events could occur at decision points where the decision is not to change the status of the system. Conversely, the system status may change continuously without an event occurring as long as these status changes have been prescribed in a well-defined manner.

Those events that occur at a specified projected point in time are referred to as time-events. They are commonly thought of in conjunction with next-event simulation. Those events that occur when the system reaches a particular state are called state-events. Unlike time-events, they are not scheduled in the future but occur when state variables meet prescribed conditions. In GASP IV, state-events can initiate time-events and time-events can initiate state-events.

The behavior of a system model is simulated by computing the values of the state variables at small time steps and by computing the values of the attributes at event times. The time step increment is automatically determined by GASP IV based on the equation form for the state variables, the time of the next event, and accuracy and output requirements.

When an event occurs, it can change the system's status in three ways: it can alter the value of state variables or the attributes of the entities; it can alter the relationships that exist among entities or state variables; or it can change the number of entities present. Any of these changes can result from the occurrence of an event. Between event times, only the values of the state variables can change and such changes must be in accordance with prescribed equations.

At each time step, the state variables are evaluated to determine if the conditions prescribing a state-event have occurred. If a state-event was passed, the step size was too large and is reduced. If a state-event occurs, the model status is updated according to the user's state-event subroutines. Step size is automatically set so that no time-event will occur within a step. This is accomplished by setting the step size so that the time-event ends the step.

Since time-events are scheduled happenings, certain attributes are associated with them. At the minimum, a time-event must have attributes that define its time of occurrence and its type.

In addition to the just described functions of providing automatic time advance, event scheduling and control, continuous variable integration with variable step size and user specified accuracy requirements, and discrete-continuous interaction procedures; GASP IV also provides subprograms that accomplish statistical data collection, random deviate generation, program monitoring and error reporting, information storage and retrieval, automatic statistical computation and reporting, standardized simulation reports, tabular and plotted histograms, automatic plotting routine, and built-in flexibility in output reports and other provided functions. Table 1 presents a list of the GASP IV subprograms and user-written subprograms that are used to accomplish these functional capabilities.

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* GASP PL/I is a PL/I version of GASP IV.[11]

Table 1. Categorization of GASP IV and User-Written Subprograms According to Functional Capability

Function	GASP IV Provided	User-written*
Time advance and status update	GASP	STATE, SCOND, EVNTS, and specific event subprograms
Initialization	DATIN, CLEAR, SET	Main program, INTLC
Data storage and retrieval	FILEM, RMOVE, CANCL, COPY, NPRED, NSUCR, NFIND	
Location of state-events	KROSS	
Monitoring of system simulation	MONTR	UMONT
Error reporting	ERROR	UERR
Data collection and reporting	COLCT, TIMST, TIMSA, HISTO, GPLOT, PRNTQ, PRNTS, SUMRY	SSAVE, OTPUT
Miscellaneous support	SUMQ, PRODQ, GTABL, GDLAY	
Random deviate generation	DRAND, UNFRM, TRIAG, RNORM, ERLNG, GAMA, BETA, NPSSN, EXPON, WEIBL, DPROB, RLOGN	

* Only those subprograms required by a specific application need be provided by the user.

Through the use of these subprograms, a GASP IV simulation model is developed. The model includes a set of event programs or state variable equations or both that describe the system's stochastic/dynamic behavior; lists and matrices that store information; an executive routine that directs the flow of information and control within the model; and various support routines.

GASP IV concepts provide a view of the world that simplifies model building. These concepts facilitate the representation of the relevant aspects of system behavior. As a programming language, GASP IV gives the computer programmer a set of FORTRAN subprograms designed to carry out the most important functions in simulation programming. Modeling concepts are translated by GASP IV into FORTRAN routines that can be easily used. GASP IV provides the link between the modeling and programming activities that is so important to a successful simulation study, as well as providing a common basis for modeling diverse systems and a well-developed framework which fosters communication between simulation modelers.

In the following sections, two examples are given that illustrate the combined modeling capabilities inherent in GASP IV as applied to environmental problems.

Simulation of Electroplating Operations [2,3,4,13,14]

Cadmium is used in the electroplating industry to provide iron and steel products with protection against corrosion. A cadmium coating also provides an attractive appearance and good solderability. The discharge of cadmium into the nation's waterways, however, poses an environmental threat in that cadmium has been associated with several chronic and acute effects in man and other species even when present in only trace amounts.

The barrel plating line simulated in this paper is represented in Figure 1. Parts to be plated are placed in large perforated barrels. Using an overhead crane, an operator lowers a barrel into the plating bath. The parts in the barrel become the cathode and attract cadmium ions from cadmium anodes which are periodically replenished by the plater. The electrolyte is composed of sodium cadmium-cyanide, excess sodium cyanide, and sodium hydroxide plus additional agents and brighteners. After a specified time, the barrel is lifted out of the bath. The parts in the barrel retain a certain volume of bath liquid at the very high cadmium concentration of the bath. This is called dragout volume and dragout concentration. The barrel is then immersed in a running rinse. Running rinses are supplied with fresh water at the bottom of the tank and empty via the overflow at the top of the tank. The dipping of a barrel causes an increase in the rinse concentration while the flowing water decreases this concentration. The next rinse is an acid bath designed to brighten plated parts with an

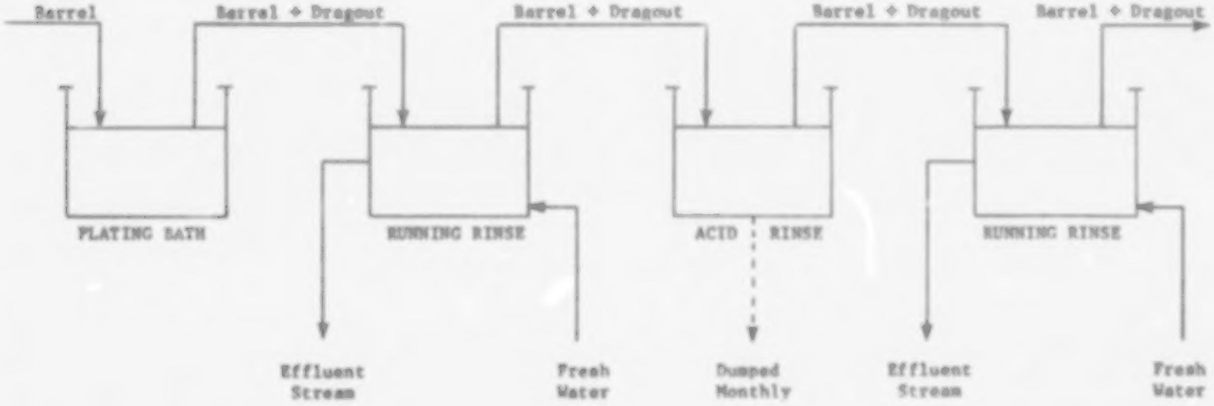

Figure 1. A Barrel Plating Line.

attractive finish. The final rinse is another running rinse. The barrels are then emptied, washed and reused. The discharge of cadmium is due to the continuous effluent flow from the running rinses and the periodic dumping of the acid rinse.

The process is modeled in terms of the events at which cadmium concentrations or equations describing these concentrations can be altered in the various parts of the process.

The insertion and removal of barrels in the rinse tanks and the dumping of tank contents are the time-events of the process. Each barrel has attributes associated with it that characterize the type of parts in the barrel, the dragout volume in the barrel, the concentration of this dragout volume, and codes denoting the next processing point (next event type) for the barrel and the time of occurrence of this event. When a barrel is placed in a running rinse, it causes a surge of effluent equal to the displacement of the barrel. The effluent due to the surge is assumed to have the current cadmium concentration of the rinse and occurs instantaneously. The barrel then immediately causes an increase in rinse concentration dependent upon the current amount of cadmium in the rinse, the volume of the rinse, and the volume and concentration of the dragout in the barrel.

The barrel stays in the rinse until it is scheduled to be withdrawn. During this stay in the rinse, the concentration of the rinse decreases due to the fresh water supply. Immediately after withdrawal, the tank begins to refill, and the concentration decreases in a different manner than when the barrel was in the tank. This is because fresh water is entering the tank but no effluent is leaving. When the tank is completely refilled, the effluent again starts pouring from the tank. Other tanks of the system are modeled in a similar fashion.

In Figure 2, a plot for one of the simulation runs of the GASP IV model of the electroplating line is presented. Time, in three minute intervals, is plotted on the independent axis. Cadmium concentration, in parts per million, and also cadmium amounts in ounces are represented on the dependent axis. The symbol 1 representing cadmium concentration in rinse tank 1 has a sawtooth behavior pattern. Increases in this variable are the result of barrel inserts into the tank. The die-away curves following the increases are the result of fresh water diluting the concentration as it enters the tank. The total process effluent is plotted using the symbol 9. As expected, the plot shows a continual increase in cadmium released as the process continues. Figure 3 shows a statistical summary of dragout volume observations made during the simulation. A histogram

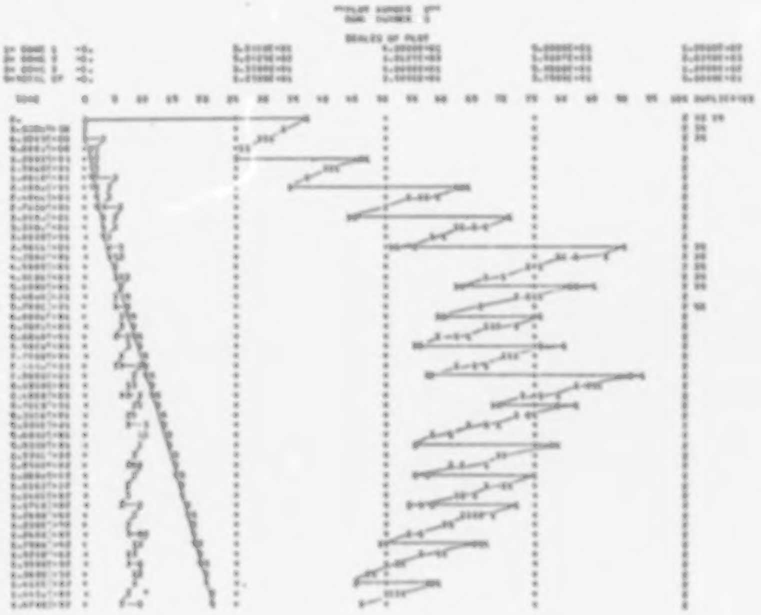

Figure 2. Plot of State Variables for Plating Line Simulation.

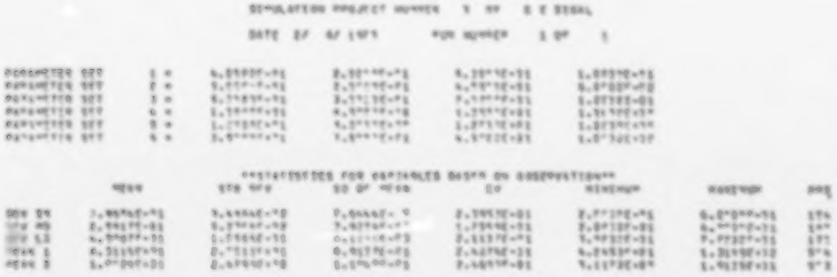

Figure 3. Statistical Summary for Plating Line Simulation.

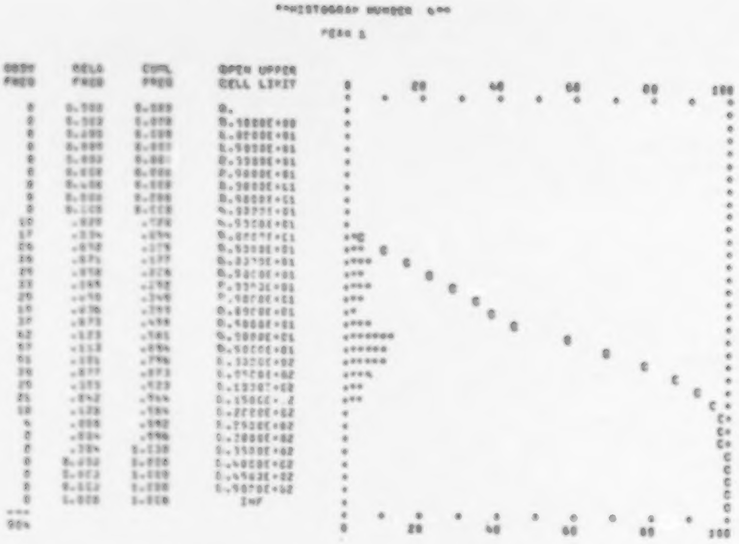

Figure 4. Histogram of Peak Cadmium Concentration of Rinse 1.

of interest to the modeler and not currently available from direct measuring procedures used is shown in Figure 4. It represents observations on peak concentration values (occurring immediately after a barrel insertion) of rinse concentration of rinse 1.

An interesting feature of this model is the tradeoff between production rate and amount of pollution in the effluent. One way to decrease the amount of cadmium in the effluent is to decrease the amount of cadmium in the dragout from the plating bath. This can be accomplished by decreasing the process flow by requiring a dwell time over the plating bath. Simulation runs were made to evaluate the tradeoffs between the increased cost due to production slow down as a basis for meeting EPA standards on cadmium concentrations in the effluent.

GASP IV Model of Cadmium Flow in an Urban Area [15]

In this example, the sixty square mile region of extreme northwestern Indiana which includes the cities of Gary and East Chicago was modeled. There are several hundred sources of cadmium emissions in the region which can be to either air or water or both. The impact of each source on the various ecosystems in the region is unclear. Questions that were raised and for which the model was designed are: 1) what are the flow patterns and characteristics of cadmium in the urban area under study?; 2) what are the levels of cadmium on urban structures?; and 3) what control policies may be useful in meeting pollution standards?

The major compartments for one portion of the model developed are shown in Figure 5. In this flowchart, the rectangles represent compartments (or levels in systems dynamics terminology), the circles represent generation rates, and the lines between circles and/or rectangles represent transfers. Equations relating the compartments to one another were developed, and these were used to define the state variables for the system. Source emission data was used in order to obtain the input components for the model. The inputs along with the equations for the state variables constitutes the continuous portion of the model. Superimposed on this continuous model are rainfall events which wash down the urban structures and provide inputs of cadmium to

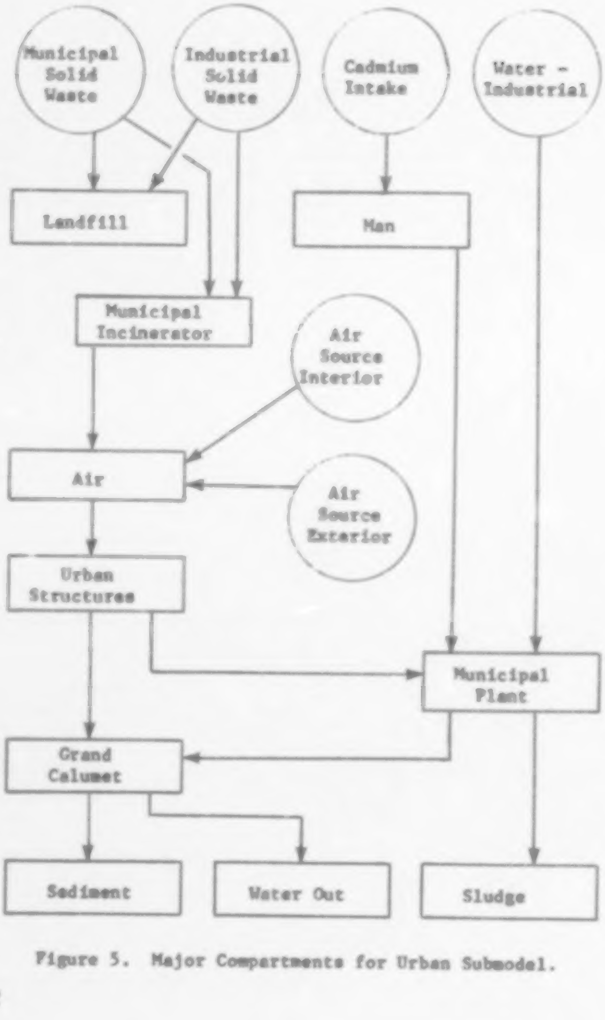

Figure 5. Major Compartments for Urban Submodel.

the municipal plant. These discrete events are significant in that they can cause overflow conditions to occur at the municipal plant. Such overflow conditions occurring at the time when cadmium and other particulate matter is washed from the urban structures could be a significant component to the levels of pollution in the waterways to which the overflow is directed.

The time behavior for each level of each compartment was obtained during the simulation. In addition, the peak values for particulate matter on the urban structures was collected along with the percent of time that the municipal plant was bypassed and the amount of pollution in the effluent that was bypassed. Sensitivity studies were performed for assessing the different rates of increase (or decrease) of total emissions and their effects on the levels of the state variables describing the system. Results from this study have been published previously.[15]

Summary

The basic concepts of combined simulation inherent in the GASP IV simulation language have been presented. The interaction between state variables, time-events, and state-events has been demonstrated through examples. The two examples presented in this paper illustrate the types of environmental systems that can be studied and analyzed using GASP IV.

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RADIONUCLIDE REMOVAL BY THE pH ADJUSTMENT OF PHOSPHATE MILL EFFLUENT WATER

David L. Norwood and Jon A. Broadway
Eastern Environmental Radiation Facility
Montgomery, Alabama 36109

Abstract

Application of the GASP IV simulation system to the waste water treatment process in a phosphate ore milling industry has been presented. Specific attention has been directed to a quantitative evaluation of precipitation of radionuclides due to the liming treatment (pH adjustment) used in a wet process plant and the residual radionuclides in effluent water. The variation in output radionuclide concentrations was studied as a function of important system parameters such as flow rate, liming rate, and pH. Extension of this modeling capability to other large industrial applications has been discussed and implications for further study have been indicated.

Introduction

A study of effluents from the phosphate mining and milling industry in Florida has been underway since 1974 by the Eastern Environmental Radiation Facility (EERF) in Montgomery, Alabama. One goal of this study has been to develop a simulation of the liming process used to treat waste water before its discharge into the environment. This liming treatment is used to adjust the pH of the waste water for the removal of flouride and phosphorous. It was shown by the EERF that radionuclides are also removed by this process.[1]

Results from further field work which will provide information on the parameters important in the radionuclide removal process will be incorporated into the model presented in this report. The objective of this study is to establish a computer model which will be helpful in estimating the radionuclides, flouride, and phosphorous which will be present in phosphate industry effluents.

Field measurements made during 1974 produced data which indicate that the liming process reduces ^{226}Ra concentrations over a range of 95% to greater than 99%. The data used in this report were collected at an operating wet process phosphoric acid plant in central Florida. An effort was made, however, to see that the model presented here is sufficiently general that it could easily be adapted to other plants which also use the liming method of pH adjustment. The parameters which characterize this model are all defined in one subroutine, which sets all initial conditions, or are set up as input values to the model.

Overview of the Effluent Treatment

The wet processing of phosphate ore involves the addition of sulfuric acid to the phosphate ore to produce gypsum and phosphoric acid. The gypsum is removed from the process water by allowing it to settle out. The process water is retained in a lake for continued sedimentation and reuse in the plant. Due to rainfall into this lake it is sometimes necessary to release some process water to the general environment. Prior to this release, the process water is routed through a series of ponds where it is treated with a lime slurry to effect pH adjustment. These ponds also allow for settling out of solids precipitated when the pH is raised. Both the raising of pH and adequate settling time are necessary for effective removal of flourides, phosphorous and radioactivity.

The treatment under consideration in this study is the double liming process used at a wet process plant in central Florida. This process consists of adding lime to the process water as it enters the system of ponds. The process water contained in the holdup pond is typically at pH of 1.5 - 3.0 before the liming treatment begins. For the purpose of the modeling process contained in this paper, the process water was assumed to be a pH of approximately 2.5 at the start of the first liming stage. Contact with the lime causes sedimentation and pH increase until the second liming occurs. The second liming stage starts at a pH of approximately 4.0 and continued contact with the lime solution causes increased sedimentation and the pH is increased to a range of 7 to 10 at the point of release to the surface water system.

Laboratory Measurement of Sedimentation Rates

One portion of this study involved a series of laboratory experiments to characterize the sedimentation rate of ^{226}Ra from the process water treated by the lime as a function of time for given values of starting pH levels. The actual process water and lime slurry as used by the phosphate plant were used in the laboratory study.

A process water sample of six liters was stirred continuously while lime was added to reach the pH value for the sedimentation study. Lime addition was stopped at a pH of 2.5 and a timer was then started to measure sedimentation rates. Samples of the supernate were removed at t = 0, 5, 10, 100, and 400 minutes for ^{226}Ra analysis by the radon emanation method as described in the American Public Health Association's Methods for the Examination of Water and Waste Water.[2] A similar experiment was performed for the second sedimentation process with a second process water sample with adjustment of the solution to an initial pH of 4.0, in order to approximate the conditions at the start of the second liming step in the industrial process. Measured concentrations of ^{226}Ra at the two initial pH levels are given in Table 1. Total ^{226}Ra in this case is the sum of the dissolved and undissolved ^{226}Ra.

Table 1

^{226}Ra Concentrations in Process Water After Liming as Measured in Laboratory Experiment

Sedimentation time after initial pH is obtained (min.)	Total ^{226}Ra for initial pH = 2.5 (pCi/l)	Total ^{226}Ra for initial pH = 4.0 (pCi/l)
0	5.5	6.6
5	2.1	8.42
10	2.94	6.62
100	1.54	0.54
400	2.16	0.42

For a given pH we have assumed that the retention rate of the radionuclides in the effluent water after treatment is dependent solely on the time spent in the liming ponds before release to the outside environment, and since the settling rate at any time is proportional to the amount of radionuclides present in the process water, we are led to an equation of the form:

$$C = C_o e^{-\lambda t} \tag{1}$$

where: t = time

C = concentration at time t,

C_o = initial concentration,

and λ = settling factor to be determined.

Using a stepwise Gauss-Newton iteration procedure on the parameters λ and C_o a non linear least square curve of the form (1) was calculated. This was facilitated by running the BMD07R program from the Bio-Medical Statistical package of programs developed by the UCLA Health Sciences Computing Facility[3] on an IBM 370 computer operated by the Optimum Systems Incorporated, of Bethesda, Maryland. This program was run once with each of the two sets of data given in Table 1. The complete results of the two runs are given in the Appendix. For an initial pH of 2.5, the procedure produced a value of $\lambda = 0.0018$, and for an initial pH of 4.0 the procedure produced a value of $\lambda = 0.020$. Although these two values need further refinement, they do give a reasonable approximation of the results obtained in actual field measurements. Further experiments can be run with an assortment of pH values in an effort to develop a single, reliable equation relating the concentration at time t to both the pH and the time spent in the liming ponds. When this final equation is determined, the model will provide a simple mechanism for estimating the effects of various combinations of liming practices at the two liming points.

GASP IV

A decision to use GASP IV as the modeling language was made because of its combined discrete/continuous modeling capabilities and because of the authors' familiarity with FORTRAN, the host language of GASP IV. Actually, the initial system presented here could have been modeled with a strictly continuous language, but future embellishments will be more easily implemented if we also have the discrete event case available.

GASP IV is a combined discrete/continuous FORTRAN based simulation language which comes to the user as a set of FORTRAN subroutines[3]. Because of its complexity, it requires more effort to use successfully than some of the other strictly discrete or strictly continuous simulation languages, however, if a model has both discrete and continuous components, then GASP IV can be well worth the extra effort. The fact that it is FORTRAN based simplifies the writing of subroutines required to customize GASP IV for the user's application and generally obviates the need to learn another high level computer language. The user has to provide subroutines (in FORTRAN) to process and schedule events and to initialize his continuous and non-GASP variables, and to allow for any additional output and/or error messages which are desired but not supplied by GASP itself.

The GASP Model

The basic model which is described in this report is an attempt to simulate the flow of liquid effluents from the process water pond through the liming ponds. We assume that the initial liming occurs at the entrance to the liming system, and that the second liming occurs somewhere between entry into the system and exit from it. For simplification, we have initially made the assumption that the system we are dealing with has reached equilibrium in the sense that the volumetric flow rate of the effluents through the system is essentially constant. As more precise information about the topography of the liming ponds is obtained we will easily be able to incorporate this into the model, but for now, only small errors will probably be induced by the assumption of constant volumetric flow rate. We have also made the assumption that the cross-section of the liming pond system at any point is a segment of a circle. This does not seem like an unreasonable assumption and it allows us to calculate the cross-sectional area from other known parameters.[4]

In setting up the GASP model for the flow of the effluents through the liming ponds it seemed that distance traversed through the liming pond system would be a more natural independent variable than actual time spent in the liming pond system. Thus, for purposes of this simulation the GASP variable TNOW was used to represent the distance that the effluent had traveled through the system. This is one indication of the adaptibility of the GASP IV simulation language. In fact, no inconsistencies at all are introduced by using distance instead of time as the independent variable. Thus, in addition to TNOW, the GASP variables TTBEG, TTLAS, TTNEX and TTFIN refer to distance from entry into the liming pond system at initial liming, the last update point, the projected next update point, and exit from the system, respectively.

The state variables SS(1) and SS(2) are used to denote the concentration at distance TNOW from entry into the liming system, and the time, in minutes, that it took to traverse the distance TNOW.

Other variables introduced into the program are VF = Volumetric Flow Rate of the effluent through the system (recall our assumption of a constant VF throughout the system), TM = elapsed time from last state event, DLIM2 = the distance from entry into the system that the second liming occurs, and a few variables which are used only in the user added FUNCTION AREA which calculates the cross-sectional area of the pond as a function of distance from entry point.

For our purposes at HERF, we have modified the original GASP IV software somewhat to achieve faster throughput and turn around of our runs, at the expense of storage for the rather large arrays which are provided with the stock version of GASP IV. A list of the arrays which can be conveniently reduced in size in this manner is provided on pages 77 and 80 of Dr. Pritsker's book, The GASP IV Simulation Language. Following is a brief discussion of each of the user written subprograms used in this model. A block diagram of their interrelationship to each other and GASP IV is given in Figure 1.

Subroutine STATE

Subroutine STATE first calculates the time increment since the last update of the concentration. Since distance is the independent variable, DTNOW gives us the distance traveled since the last update. Thus, if we know the volumetric flow rate and the average cross-sectional area of the ponds over that distance we can easily calculate the time lapse, (TM) by

$$\mathrm{TM} = \mathrm{DTNOW} * \mathrm{AREA}(X)/\mathrm{VF} \tag{2}$$

where AREA(X) = cross-sectional area at distance X from initial liming

and $\mathrm{TTLAS} \le X \le \mathrm{TNOW}$.

Volumetric flow rate is initialized in Subroutine INIT and is considered constant throughout the system and the cross-sectional area is calculated in FUNCTION AREA.

Function Area

The basic assumptions made in calculating the cross-sectional area of the pond system is that the cross-section is a segment of a circle. We are then able to get the cross-sectional area if we can get the chord of this segment of a circle and the perpendicular distance from the chord to the arc of the segment by using the law of cosines to get the radius and applying the standard formula for area of a segment of a circle.[4] The chord is just the width of the liming pond at that point and since the ponds are kept dredged to a depth of about 7 feet, that suffices as the other measurement.

Subroutine INTLC

The initial conditions subroutine is used to input the initial values for the volumetric flow rate (VF), distance at which the second liming occurs (DLDM2), and the initial concentration (SS(1)), and the initial time (SS(2)).

Subroutine SSAVE

This subroutine is used to tell the GASP IV executive which variables (in this case distance, TNOW, and time, SS(2)) are to be plotted by the GASP IV provided plot routine.

Conclusions

Three simulations have been run at this time using three different volumetric flow rates. The results of using a typical low VF of 10.6 m^3/min, and "average" VF of 16.0 m^3/min and a high VF of 38.9 m^3/min are shown in Figure 2. From these three outputs the effect of modifying the volumetric flow rate is obvious. The higher the flow rate, the less time the water spends in the liming system and consequently the more radionuclides that are released to the environment. Obviously there is an optimal VF somewhere since a stagnant liming pond system (VF = 0) is clearly not ideal. As more information is gathered concerning the phosphate plant release to the process water pond and their behavior in that pond, this model can be used to determine the optimal VF.

This model is only a first step in the process of simulation removal of radionuclides from the effluents of a phosphate plant. However, with this basic model and the discrete/continuous capabilities of GASP IV more complex functions such as seasonal effects and discrete lime addition can be included. Such refinements will increase the model's effectiveness as a tool in the evaluation of the release of radionuclides into the environment from phosphate plants using the liming procedure.

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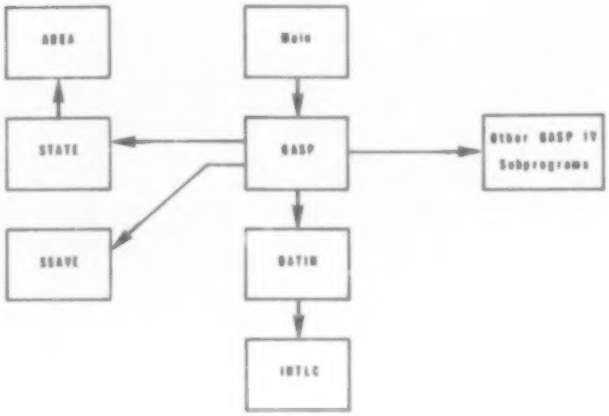

Relation of Subprograms in model

A → B = Subprogram A calls Subprogram B.

Subroutine GASP is the GASP IV provided executive subroutine
and subroutine DATIN is the GASP IV provided data input subroutine.
Figure 1.

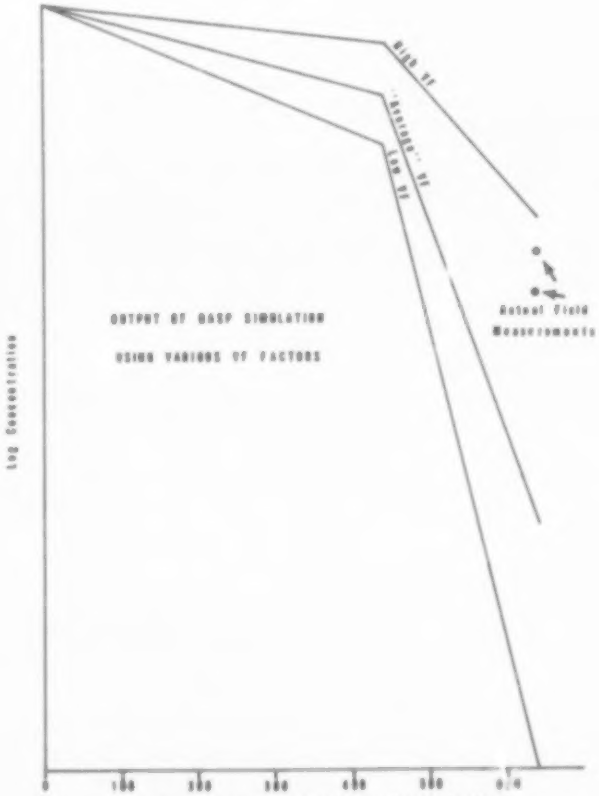

Figure 2. Distance From First Liming (meters)

APPENDIX

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BMDX85 - NON LINEAR LEAST SQUARES - REVISED NOVEMBER 19,1971

HEALTH SCIENCES COMPUTING FACILITY, UCLA
PROBLM CODE                           PH4.0
NUMBER OF VARIABLES                       2
INDEX OF THE DEPENDENT VARIABLE           2
INDEX OF THE WEIGHTING VARIABLE           0
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NUMBER OF PARAMETERS                      2
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EPSILON                             0.000010
MAXIMUM NUMBER OF ITERATIONS        100
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              SQUARE
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    2  0   1.2617E 00   7.8361E 00 -1.9339E-02
    3  0   1.2604E 00   7.8625E 00 -2.0017E-02
    4  0   1.2602E 00   7.8521E 00 -1.9760E-02
    5  0   1.2602E 00   7.8563E 00 -1.9866E-02
    6  0   1.2602E 00   7.8546E 00 -1.9824E-02
    7  0   1.2602E 00   7.8553E 00 -1.9841E-02
    8  0   1.2602E 00   7.8550E 00 -1.9834E-02
    9  0   1.2602E 00   7.8552E 00 -1.9837E-02
   10  0   1.2602E 00   7.8551E 00 -1.9836E-02
ASYMPTOTIC STANDARD DEVIATIONS OF THE PARAMETERS

           8.0854E-01  9.8005E-03
ASYMPTOTIC CORRELATION MATRIX OF THE PARAMETERS
           1           2
  1       1.00000     -0.48216
  2      -0.48216      1.00000
CASE        F            Y-F  STANDARD              VARIABLES
                              DEVIATION
                              OF ESTIMATE
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   2     7.11343      1.30656     0.64148      5.00000        8.42000
   3     6.44178      0.17822     0.65921     10.00000        6.62000
   4     1.08066     -0.54066     1.01017    100.00000        0.54000
   5     0.00281      0.41719     0.01089    400.00000        0.42000
```

```
BMDX85 - NON LINEAR LEAST SQUARES - REVISED NOVEMBER 19,1971

HEALTH SCIENCES COMPUTING FACILITY, UCLA
PROBLM CODE                     PH 2.5
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INDEX OF THE WEIGHTING VARIABLE     0
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EPSILON                          0.000010
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REWIND OPTION                     NO
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             SQUARE
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    2  0   2.7034E 00  3.2648E 00 -1.5529E-03
    3  0   2.6962E 00  3.2917E 00 -1.7475E-03
    4  0   2.6956E 00  3.3002E 00 -1.8051E-03
    5  0   2.6955E 00  3.3027E 00 -1.8217E-03
    6  0   2.6955E 00  3.3034E 00 -1.8263E-03
    7  0   2.6955E 00  3.3036E 00 -1.8277E-03
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   10  2   2.6955E 00  3.3037E 00 -1.8282E-03
ASYMPTOTIC STANDARD DEVIATIONS OF THE PARAMETERS

           9.2291E-01  2.6167E-03
ASYMPTOTIC CORRELATION MATRIX OF THE PARAMETERS
           1           2
   1      1.00000    -0.42726
   2    -0.42726      1.00000
CASE       F            Y-F  STANDARD           VARIABLES
                             DEVIATION
                             OF ESTIMATE
   1     3.30371     2.19629     0.92291     0.0         5.50000
   2     3.27365    -1.17365     0.89705     5.00000     2.10000
   3     3.24386    -0.30386     0.87330    10.00000     2.94000
   4     2.75173    -1.21173     0.79775   100.00000     1.54000
   5     1.59007     0.56993     1.52825   400.00000     2.16000
```

AN APPLICATION
OF BIASED ESTIMATION THEORY
TO ITERATIVE MAXIMUM LIKELIHOOD SEARCH STRATEGIES

David J. Svendsgaard
Mathematical Statistician
Health Effects Research Laboratory
U. S. Environmental Protection Agency
Research Triangle Park, North Carolina

Summary

In scientific investigations, bias is generally regarded as something that is not wanted. In theoretical statistics, biased estimation has been studied with a view toward obtaining improved estimators. Often times, such improved estimators require subjective input from the investigator — another something that is not generally accepted in scientific investigations. This paper documents a situation where the use of biased estimation works better than unbiased estimation. Although we believe the situation is important in its own right, we consider it as evidence that biased estimation theory deserves serious consideration in environmental modelling work.

Here, we describe a modification to an existing iterative scheme for obtaining the maximum likelihood estimators of the parameters of the cumulative logistic function adjusted for natural responsiveness. This modification incorporates the concept of biased estimation, while the original scheme is viewed as using unbiased estimation. Empirical results indicate that a higher percentage of successful convergences occur when the modification is used. We believe that the modification [illegible] less dependent on the starting values, and that the modification requires subjective input in a form that is easy for most potential users to specify.

We conclude our discussion with comments on the fitted dose-response model.

Introduction

Background

Parametric dose-response models have great utility in quantifying the relationship between an agent and a health effect of that agent. Knowledge of such relationships is key information for the determination of air quality standards.

The parameters of such models are estimated from observed data. The maximum likelihood estimators (MLE) of these parameters have good statistical attributes, and so the MLE is often calculated. Even for simple mathematical models, this calculation usually involves the use of iterative methods. Such iterative schemes do not always successfully converge to the MLE.

We have attempted to determine the MLE for the cumulative logistic function adjusted for natural responsiveness. The data was obtained in an epidemiological panel study. Generally, there are no control groups for such studies and existing iterative methods can perform poorly under such circumstances. Difficulty in using one such method was experienced in this case.

The success of the iterative method we used depended heavily on our ability to start the iteration with good starting estimates of the parameters (starting values). If one set of starting values doesn't result in convergence, one tries another set. Complex subjective judgments may be required to obtain good starting values. Since starting with the MLE as a set of starting values will usually result in convergence, one can always be accused of using poor starting values when the iterative scheme fails.

Statement of the Problem

There are a couple of ways that an iterative scheme can fail. When very poor starting values are used, convergence to a relative maximum may take place, or the specified number of iterations may be used up before convergence to the MLE has occurred. Another type of failure results when the revised estimates overshoot the MLE and get progressively worse. This type of failure occurs when a certain matrix requiring inversion is ill-conditioned. It is this type of failure that was experienced in our case, and it is this type of problem that our modification is designed to handle.

Biased Estimation

This type of failure can be viewed as the fault of unbiased estimation. At each iteration the revised estimates are derived from a solution vector. This solution vector can be considered the least squares estimator of the parameters of a particular linear model. Although the least squares estimator attains minimum variance among unbiased estimators, this variance can be large.

The theory of biased estimation is based on the fact that mean squared error (bias plus variance) can be smaller for a slightly biased estimator with much smaller variance, than for an unbiased estimator. This theory is applied to develop a class of estimators appropriate for this problem. The result is an iterative maximum likelihood search strategy in which the user of the method simply specifies a bound on the difference between the MLE and the starting value for the proportion of natural responses. The method using the least squares estimator can be viewed as considering this difference to be unbounded. Thus, the user can specify a very crude bound and expect to do better by incorporating this bound into the modified method.

Overview

First, we present the theory involved. This includes a description of the dose response model, a description of the iterative method, the development of a modification to this iterative method, and a discussion on the subjective input required to use the modification.

Second, we do an empirical evaluation of this modification. The data used in the evaluation is described. Next, we describe the evaluation, list the results, and draw conclusions.

Finally, we make some comments on the application of this model when it is fitted to epidemiological panel studies.

Theoretical Development

Description of the Cumulative Logistic Adjusted for Natural Responsiveness Dose-Response Model

Consider a dose-response experiment where dose levels Z_i at N different levels are applied to n_i subjects and at each dose level r_i subjects respond.

If the administration of a dose Z causes a proportion P(Z) of the test subjects to respond and other independent factors acting on the test subjects during the experiment causes a proportion C to respond, then the total expected proportion responding will be

$$P'(Z) = P(Z) + C - P(Z)C = C + (1 - C)\,P(Z). \qquad (1)$$

This equation is called Abbott's Formula. If P(Z) is the cumulative logistic function

$$P(Z) = \frac{1}{1 + \exp - (A+BZ)}$$

then P'(Z) is known as the cumulative logistic adjusted for natural responsiveness.

Tolerance Concept

This model is motivated by the concept of a tolerance. An individual's tolerance is defined as that level of dose Z_0 such that doses higher than Z_0 always cause a response. The purpose of the model is to make inferences about the distribution of tolerances in a target population.

Sampling Considerations

In fitting such models, it is usual to assume that the n_i subjects exposed to a dose level Z_i were randomly selected from the target population. Assume in addition that the proportion of tolerances less than Z is P(Z) for each Z. When these two assumptions are correct the probability of observing r_i responses from the n_i subjects dosed at level Z_i for i=1,2,...,N is

$$L(A,B,C) = \prod_{i=1}^{N} \binom{n_i}{r_i} P(Z_i)^{r_i} (1-P(Z_i))^{n_i-r_i}.$$

In general, L(A,B,C) is called the likelihood function. Those choices of A, B, and C (denoted by $\hat{A}$, $\hat{B}$, and $\hat{C}$) that maximize L(A,B,C) are the MLE.

Description of an Existing Iterative Method

Based on an approximation to the first derivative of the log likelihood evaluated at the MLE by the first order terms of the Taylor-Maclaurin expansion, Finney[1] has derived the expressions used in iteratively solving for the MLE of the parameters of the probit dose-response model adjusted for natural responsiveness. These expressions can be easily applied to the logistic model described in (1). When A_s, B_s and C_s are the starting values for the parameters A, B, and C respectively, at the iteration number S, the revised estimates $(A_{s+1}, B_{s+1}, C_{s+1})$ are

$$\begin{bmatrix} A_{s+1} \\ B_{s+1} \\ C_{s+1} \end{bmatrix} = \begin{bmatrix} \hat{\alpha}_o \\ \hat{\alpha}_1 \\ \hat{\alpha}_2 + C_s \end{bmatrix}$$

The formulae for $\hat{\alpha}_o$, $\hat{\alpha}_1$ and $\hat{\alpha}_2$ are algebraically the same as the formulae for the least squares estimator of the parameters of the linear model

$$y_i = \alpha_o x_{oi} + \alpha_1 x_{1i} + \alpha_2 x_{2i} + \varepsilon_i \qquad (2)$$

for i=1,2,...,N;
where the ε_i are uncorrelated random variables with zero mean and common variance σ^2. The x_{oi}, x_{1i}, and x_{2i} are all determined from A_s, B_s and C_s, and the formula for the y_i also involves r_i. The formulae below define the x_{ji} and y_i for i=1,2,...,N and j=0,1 and 2.

$$\hat{P}_i = \frac{\frac{r_i}{n_i} - C_s}{1 - C_s};$$

$$P_i = \frac{1}{1 + \exp - (A_s + B_s Z_i)};$$

$$Q_i = 1 - P_i;$$

$$W_i = P_i Q_i;$$

$$w_i = \frac{W_i^2}{Q_i\left(P_i + \frac{C_s}{1-C_s}\right)};$$

$$y_i = \left(A_s + B_s Z_i + \frac{\hat{P}_i - P_i}{W_i}\right) (n_i w_i)^{\frac{1}{2}};$$

$$x_{oi} = (n_i w_i)^{\frac{1}{2}};$$

$$x_{1i} = Z_i\,(n_i w_i)^{\frac{1}{2}};$$

and $x_{2i} = \frac{Q_i}{W_i} (n_i w_i)^{\frac{1}{2}}$.

If C_1 is obtained from inspection of the data, A_1 can be obtained by iteration to maximize the likelihood for this value of C_1. The appropriate expressions involved in this first stage of iteration are algebraically equivalent to the least squares estimators

$$\begin{bmatrix} \hat{\alpha}_o \\ \hat{\alpha}_1 \end{bmatrix} = \begin{bmatrix} A_1 \\ B_1 \end{bmatrix}$$

for the parameters of the model

$$y_i = \alpha_o x_{oi} + \alpha_1 x_{1i} + \varepsilon_i, \qquad i=1,2,\ldots,N; \qquad (3)$$

which is obtained from (2) by setting α_2 to zero. Of course, starting values for A and B are required even for this first stage of iteration, and for B_o one could use zero and set

$$A_o = \ln \frac{\overline{P}-C_1}{1-\overline{P}},$$

where $\overline{P} = \frac{\Sigma r_i}{\Sigma n_i}$.

This choice of starting value for A_o maximizes the likelihood function for these values of B_o and C_1. Having obtained revised estimates for A and B after a number of iterations from this first stage, one could proceed to the second stage of iteration using (2) and these revised estimates as starting values.

Based on empirical results, it appears that the success of such a two stage scheme depends on how well C_1 is chosen and on what criterion is used to determine when to stop first stage iterations and go to the second stage. A very stringent criterion is wasteful of computer time if C_1 is chosen close to $\hat{C}$. When a very loose criterion is employed, e.g. omitting the first stage entirely, failure rates are high. The failures are usually the result of high correlations among the x_{ji} resulting in a singularity in the matrix requiring inversion. Invariably, such a singularity is preceded by an unreasonably large overestimation of the magnitude of α_2.

When we regard (2) as the true model whose parameters are to be estimated, the problems mentioned in the last paragraph are a familiar weakness of least squares estimation. That is, even though the least squares estimator achieves minimum variance among unbiased estimators, this variance can be very large when the independent variables are highly correlated. In those cases cited above, we view this variance as being intolerably large. Possibly a slightly biased estimator with much smaller variance can achieve small enough mean squared error (bias plus variance) to usually avoid those type of problems.

Development of an Alternative Estimator via the Consideration of Biased Estimation Theory

Consider the class of biased estimators of the form

$$\begin{bmatrix} a_o \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \bar{\alpha}_o \\ \bar{\alpha}_1 \\ 0 \end{bmatrix} + \begin{bmatrix} k_o \\ k_1 \\ k_2 \end{bmatrix} \hat{\alpha}_2, \qquad (4)$$

where k_o, k_1 and k_2 are constants. We shall consider using the a_i in place of the $\hat{\alpha}_i$ in a single phase iteration scheme. Note if the k_i are zero then the a_i are the least squares estimators of the model described in (3) which are biased when α_2 is nonzero. It is also possible to obtain the $\hat{\alpha}_i$ from (4) by letting the k_i take on certain values.

We shall use an error criterion that seems appropriate for this problem and show how the k_i can be chosen so that for a wide range of α_2 values, better performance in terms of this criteria is attained by an estimator using the chosen k_i's than is attained by using either of the estimators mentioned in the above paragraph. The choice of the k_i is made by specifying an upperbound on α_2^2/σ^2.

It turns out that the formula for the k_i that we suggest using involves the specified upperbound and the correlation between the x_{ji}. Generally, this correlation changes from one iteration to the next, so that even though only one bound is used, the k_i vary between iterations. In those cases where successful convergence takes place, the estimators are similar to those that were suggested for the two stage scheme. Initially, the x_{ji} are highly correlated and the k_i are zero. In later iterations, the correlations become smaller and the a_i's approach the $\hat{\alpha}_i$'s. Thus, instead of selecting a criteria for deciding when to jump from the first to second stage of iterations, the use of the proposed estimator eliminates the need to make this decision by automatically incorporating it into the computation process based on the value of the specified upperbound.

Let the true model at each iteration be

$$\eta=\alpha_o x_o+\alpha_1 x_1+\alpha_2 x_2,$$

and consider approximating η over an interval of interest $\xi_o \le x \le \xi_1$ with

$$\hat{\eta}=a_o x_o+a_1 x_1+a_2 x_2$$

where (a_o, a_1, a_2) is a vector of estimated regression coefficients. A reasonable measure of the closeness of $\hat{\eta}$ to η is integrated mean square error

$$J=\frac{N\Omega}{\sigma^2}\int_{\xi_o}^{\xi_1} E\ (\hat{\eta}-\eta)^2 \quad dx$$

where $\Omega^{-1}=\int_{\xi_o}^{\xi_1} dx$. Note that $J=B+V$,

where $B=\frac{N\Omega}{\sigma^2}\int_{\xi_o}^{\xi_1} (E(\hat{\eta})-\eta)^2 \ dx$,

and $V=\frac{N\Omega}{\sigma^2}\int_{\xi_o}^{\xi_1} \mathrm{Var}\ \hat{\eta}\ dx.$

Let $\underset{\sim}{Y}$ be the vector whose ith element is y_i and denote the design matrix whose ith row is (x_{oi}, x_{1i}, x_{2i}) by

$$\underset{N\times 3}{\underset{\sim}{X}} = [\underset{N\times 2}{\underset{\sim}{X_1}} \ \vdots \ \underset{N\times 1}{\underset{\sim}{X_2}}];$$

then

$$E(\underset{\sim}{Y})=\underset{\sim}{X_1}\begin{bmatrix} \alpha_o \\ \alpha_1 \end{bmatrix}+\underset{\sim}{X_2}\alpha_2,$$

and $\mathrm{Var}\ \underset{\sim}{Y} = \sigma^2 I_N$.

We shall consider the class K of estimators of the general form in (4)

where

$$\begin{bmatrix} \bar{\alpha}_o \\ \bar{\alpha}_1 \end{bmatrix} = (\underset{\sim}{X_1'}\underset{\sim}{X_1})^{-1}\underset{\sim}{X_1'}\underset{\sim}{Y}$$

and $\hat{\alpha}_2=(\underset{\sim}{X_2'}\underset{\sim}{H}\underset{\sim}{X_2})^{-1}\underset{\sim}{X_2'}\underset{\sim}{H}\underset{\sim}{Y}$

where $\underset{\sim}{H}=\underset{\sim}{I_N}-\underset{\sim}{X_1}(\underset{\sim}{X_1'}\underset{\sim}{X_1})^{-1}\underset{\sim}{X_1}$.

Now

$$E\begin{bmatrix} \bar{\alpha}_o \\ \bar{\alpha}_1 \end{bmatrix} =(\underset{\sim}{X_1'}\underset{\sim}{X_1})^{-1}\underset{\sim}{X_1'}\underset{\sim}{X}\begin{bmatrix} \alpha_o \\ \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} \alpha_o \\ \alpha_1 \end{bmatrix} + \begin{bmatrix} \mu_o \\ \mu_1 \end{bmatrix} \quad \alpha_2$$

where

$$\begin{bmatrix} \mu_o \\ \mu_1 \end{bmatrix} = (\underset{\sim}{X}_1'\underset{\sim}{X}_1)^{-1}\underset{\sim}{X}_1\underset{\sim}{X}_2$$

and $E(\hat{\alpha}_2)=\alpha_2$.

Denote

$$\underset{3x3}{\underset{\sim}{W}} = \begin{bmatrix} \underset{\sim}{W}_1 & \underset{\sim}{W}_2 \\ 2x2 & 2x1 \\ \underset{\sim}{W}_2' & \underset{\sim}{W}_3 \\ 1x2 & 1x1 \end{bmatrix} = \Omega \int_{\xi_o}^{\xi_1} \begin{bmatrix} x_o \\ x_1 \\ \hline x_2 \end{bmatrix} [x_o, x_1 \,\vdots\, x_2]\, dx,$$

$$\underset{\sim}{\mu} = \begin{bmatrix} -\mu_o \\ -\mu_1 \\ 1 \end{bmatrix} \text{ and } \underset{\sim}{k} = \begin{bmatrix} k_o \\ k_1 \\ k_2 \end{bmatrix}$$

The integrated mean square error of estimators in K is

$$J(\underset{\sim}{k}) = \frac{N}{\sigma^2}\alpha_2^2(\underset{\sim}{k}-\underset{\sim}{\mu})'\underset{\sim}{W}(\underset{\sim}{k}-\underset{\sim}{\mu}) + N \text{ trace } \underset{\sim}{W}_1(\underset{\sim}{X}_1'\underset{\sim}{X}_1)^{-1}$$

$$+ N \text{ trace } \underset{\sim}{W}\, \underset{\sim}{k}'(\underset{\sim}{X}_2'\underset{\sim}{H}\underset{\sim}{X}_2)^{-1}\underset{\sim}{k}.$$

When $\underset{\sim}{k}=\underset{\sim}{\mu}$, the estimator is unbiased and when $\underset{\sim}{k}=\underset{\sim}{0}$, V is smallest for any estimator in K. Differentiating $J(\underset{\sim}{k})$ with respect to $\underset{\sim}{k}$ and setting the derivatives to zero yields that the minimum J estimator in K is

$$\begin{bmatrix} \tilde{\alpha}_o \\ \alpha_1 \\ 0 \end{bmatrix} + \underset{\sim}{k}^* \hat{\alpha}_2$$

where

$$\underset{\sim}{k}^* = \frac{\alpha_2^2/\sigma^2}{\alpha_2^2/\sigma^2 + (\underset{\sim}{X}_2'\underset{\sim}{H}\underset{\sim}{X}_2)^2}\,\underset{\sim}{\mu}.$$

This value of $\underset{\sim}{k}$ requires that one know α_2^2/σ^2, but using

$$\underset{\sim}{k}^+ = \max\left(0, \frac{M-(\underset{\sim}{X}_2'\underset{\sim}{H}\underset{\sim}{X}_2)^{-1}}{M+(\underset{\sim}{X}_2'\underset{\sim}{H}\underset{\sim}{X}_2)^{-1}}\right)\underset{\sim}{\mu}$$

it can be shown that

$$J(\underset{\sim}{k}^+) < \min\,(J(\underset{\sim}{0}), J(\underset{\sim}{\mu})) \tag{5}$$

$$\text{when } \frac{M-(\underset{\sim}{X}_2'\underset{\sim}{H}\underset{\sim}{X}_2)^{-1}}{M(\underset{\sim}{X}_2'\underset{\sim}{H}\underset{\sim}{X}_2)+3} < \frac{\alpha_2^2}{\sigma^2} < M. \tag{6}$$

So if $\underset{\sim}{k}^+$ is obtained by specifying any value for M such that (6) is true, smaller J will be achieved using (a_o, a_1, a_2) with $k=k^+$ then when $k=0$ or μ.

Considerations on Choosing M

One way to choose a value M that bounds α_2^2/σ^2 is to find an upper bound for α_2^2 and a lower bound for σ^2. Therefore, first consider α_2 as being $C-C_s$, since $C_{s+1} = \bar{\alpha}_2 + C_s$. Partial justification for considering $\alpha_2 = C-C_s$ can be based on a result from large sample theory: "...if first approximations are of nonzero efficiency, one cycle of computation will yield fully efficient estimates".[1] By (1), C is a proportion so if we agree to set C_1 to some value between zero and one then $(C-C_1)^2 = \alpha_2^2$ will be less than one.

Considering only the variability contributed to y_i by $\bar{P}_i$ we have

$$\sigma^2 = \text{Var } y_i = \frac{(1-C)\ (C+(1-C)P_i(1-P_i)}{(1-C_s)\ (C_s+(1-C_s)P_i(1-P_i)}.$$

When we assume that the starting values are equal to the respective true parameters of the model, we have that σ^2 is one. For these reasons we suggest using M=1.

Smaller values for M such as $\bar{P}_1^2$ might be used, but we have only shown that (6) is true when (5) is true for the case where k is deterministic. The use of any information gained from the data in fixing $\underset{\sim}{k}$ would require that k be treated as random.

Actually, considering the error criterion we are using, even when M is carefully chosen the error may be unacceptably large. So if the iteration routine fails one should consider varying M, however choosing M larger than 1 seems unnecessary.

Empirical Evaluation of Modification

Description of the Data Used in Evaluating the Itera-Methods

Hammer et al[2] reported on data from student nurses in Los Angeles who completed daily symptom diaries during the period of their training. The total number of yes/no responses of four symptom categories pooled over days having the same range of maximum hourly oxidant levels were computed from Table 3 of this reference. The doses were the midpoints of these oxidant ranges. The symptom categories are Headache, Eye Discomfort, Cough and Chest Discomfort with no accompanying fever, chills or temperature. Due to the restrictions, the positive responses are indicators of only mild personal discomfort.

Assuming independence between days of responses from the same student nurse, the number of positive responses are taken to be binomially distributed with parameters P_i' and n_i where

$$P_i' = C + (1-C)/(1+\exp-(A+BZ_i) \text{ for } i=1,2,\ldots,9.$$

The MLE's for the parameters (A, B, C) of this model are listed in Table I for each symptom. The i's are ordered so that Z_1 is the lowest oxidant range and Z_9 is the highest.

Description of Evaluation

Iterations were run using three different starting values for C and four different bounds on α_2^2/σ^2. The starting values for C were:

(a) The observed proportion of total responses corresponding to the lowest oxidant level. For all four symptom categories this proportion turned out to differ from the MLE for C by less than 0.01. The minimum observed proportion was used as a starting value for C in the case of Chest Discomfort in order to avoid the computation of the logarithm of a negative number in the process of getting a starting value for A.

(b) One half the proportion used in (a).

(c) Zero.

The starting value for B was zero and the starting value for A was

$$A_s = \ln (\overline{P}-C_s)/(1-\overline{P})$$

where $\overline{P} = (\Sigma r_i)/\Sigma n_i$.

The four different values for M used were $\hat{P}_1^2$, $\hat{P}_9^2$, 1, and ∞. Infinity corresponds to using the least squares estimator for (2).

Iterations were continued until the change in the likelihood was zero (to the accuracy of the computer), or until 30 iterations, or until the program faulted. The maximum number of iterations was 25.

Table I

Maximum Likelihood Estimates for Each Symptom

Symptom	$\hat{A}$	$\hat{B}$	$\hat{C}$
Headache	-4.6269	.0407	.0954
Eye Discomfort	-5.0457	.0931	.0417
Cough	-9.9495	.1690	.0944
Chest Discomfort	-13.2602	.2243	.0177

Results

Table II lists the occurences of successful convergence. From this table it can be seen that the percent of successful conversions was higher in all cases when a finite bound on α_2^2/σ^2 was used. When $\hat{P}_1^2$ was specified as a bound, the failure was due to convergence to the MLE of A and B for the starting value C_1. The highest percent of successful conversions when a starting value for C of either 0 or $1/2\hat{P}_1$ was used occurred when M was set equal to one.

Conclusions

If good starting values are used, convergence can always take place using Finney's formula. However, how good these starting values must be depends on the data.

The modification of Finney's formula developed here yields successful convergence for starting values that are too poor to be used directly in Finney's formula. When very poor starting values for C are used neither the modification nor Finney's formula works all the time. However, for some values of M, a higher success rate can be obtained using the modification. Moreover, when seemingly adequate C starting values are used, successful convergence is obtained using the modification in cases where the use of Finney's formula had failed.

The use of smaller M values seems to yield poorer success rates for poor choices of C starting values, but can achieve improved success rates for seemingly adequate C starting values.

It is recommended that a number of C starting values be used with this modification. When no other information is available, M should be taken to be one. If convergence fails due to a singularity, a tighter bound should be tried. A plot of the likelihood obtained at the final iteration versus the corresponding C value is helpful for deciding if more starting values should be tried and what values to use.

Table II

Successful (S) and Failing (F) Iteration Attempts

M	Symptom	Starting Value for C		
		o	$\frac{1}{2}\hat{P}_1$	$\hat{P}_1$
$\hat{P}_1^2$	Eye Discomfort	S	S	S
	Headache	F	F	S
	Cough	F	F	S
	Chest Discomfort	F	F	S
	% Success	25	25	100
$\hat{P}_9^2$	Eye Discomfort	S	S	F
	Headache	F	F	S
	Cough	F	F	S
	Chest Discomfort	F	F	F*
	% Success	25	25	50
1	Eye Discomfort	S	S	F
	Headache	S	S	S
	Cough	F	F*	S
	Chest Discomfort	F	F*	F*
	% Success	50	50	50
∞	Eye Discomfort	F*	F*	F*
	Headache	F*	F*	F*
	Cough	F*	F*	S
	Chest Discomfort	F*	F*	F*
	% Success	0	0	25

* Indicates failure occurred due to program default.

Some Comments on Applications of Dose-Response Model When Fitted to Data From Panel Studies

Both the logistic and the probit models were fit to the Nurse eye discomfort data. The fit of both models was almost identical. The Probit fit just a little better, but the difference in fit provided no substantial grounds for choosing between the models. The adjustment for natural responsiveness was significantly different from zero ($p \leq 0.05$). There was also significant lack of fit ($p \leq 0.05$) for both models. A test of equal proportions reporting eye discomfort on days having the same maximum oxidant reading was also rejected.

It is felt that these models when adjusted for natural responsiveness adequately describe the relationship between eye discomfort and oxidant measurements for these nurses. The fact that there was significant lack of fit for these models is attributed to dose error resulting probably from spatial variation. That is, the fixed air sampler is only a crude indicator of dose for these nurses.

For purposes of selecting an air quality standard, it is felt that this modelling effort is sufficient.

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ECONOMIC AND DEMOGRAPHIC MODELING RELATED TO ENVIRONMENTAL MANAGEMENT

Allen V. Kneese, Professor, Department of Economics
University of New Mexico, Albuquerque, New Mexico 87131

Summary

I will select a few main modeling issues for discussion. First, economic-social-environmental problems are accumulating at a great rate. As a consequence, I fear that there will be a great temptation to apply models to complex issues when, in fact, they are not well designed to deal with them, and then to base policy on conclusions which may be quite unrealistic. Second is the old but still very important issue of how far one should carry the explicit incorporation of interdependencies in models, and the related question of whether one is better advised to use optimization or simulation approaches and under what circumstances.

I will conclude the paper by discussing an optimization model designed to test a number of hypotheses about quantitative modeling and the environment. From these hypotheses I will single out one which I feel is currently of particular importance to the Environmental Protection Agency. When EPA was formed, a main rationale was that the environmental media, the land, the water, the air, should be treated simultaneously in the policymaking and administrative process. This has not occurred, and I wish to indicate evidence concerning its importance and to discuss the role of a formal quantitative model in generating this evidence.

Introduction

"But I deeply fear a much worse outcome. We are seeing a proliferation of costly attempts to establish environmental management 'data banks' containing everything up to and including the kitchen sink. These are to be linked by some forms of vaguely specified models constructed by loosely organized interdisciplinary and interuniversity teams. When these huge jerry-built structures come crashing down, as many of them surely must, we may well see a backlash on the part of sponsoring agencies deeply embarrassed by their inability to show useful results from enterprises which have run into the millions of dollars. This may mean that all economic ecological modeling enterprises become discredited, even sober and well thought through ones. If this happens, it could greatly retard the further successful application of management science to this important area of national concern."[1]

The paper from which the above quote is taken was published in 1973 but was written in 1970. It was in response to the euphoria and enthusiasm about mathematical modeling applied to social problems which characterized the latter part of the 1960's. Most unfortunately, the fears expressed in this paper have come true. Today, to mention mathematical modeling in proposals going to the NSF-RANN program for funding is the end of the proposal. We hold this conference in an atmosphere characterized by enormous skepticism about mathematical modeling in general and about large quantitative models in particular. The skepticism is a reaction to a number of things: the exaggerated claims which have been made for modeling, modeling without data, indulging in the circular reasoning of drawing conclusions about the real world from assumed relationships in models, specification of irrelevant objective functions, the definition of "systems" which correspond to no present or potential decisionmaking unit, and so forth. One result has been the creation of a number of models which, at worst, produced results that are deceptive or, at most, are useless and costly. This is not to say that there have not been some notable successes, but at the moment we are suffering heavily from past mistakes.

Asking Models Questions They Were Not Designed To Analyze

Attitides toward models in the natural resources and environmental area tend to fall at polar extremes; on the one hand are the totally skeptic and on the other those who uncritically accept whatever data a model produces. As an example of the latter, the recent Ford Foundation Energy Report is a case in point. Among other things, the Ford Energy Report incorporated a mathematical projections model to answer questions about the economic effects of reduced rates of energy use. Before discussing projections, a quote from Mark Twain creates the proper mood for attempting a long-range look into the future.

"In the space of one hundred and seventy-six years the Lower Mississippi has shortened itself 242 miles. That is an average of a trifle over one mile and a third per year. Therefore, any calm person who is not blind or idiotic, can see that in the old Oolitic Silurian Period, just a million years ago next November, the Lower Mississippi River was upward of one million three hundred thousand miles long. By the same token any person can see that seven hundred and forty-two years from now the Lower Mississippi will be only a mile and three quarters long. There is something fascinating about science. One gets such wholesale returns of conjecture out of such a trifling investment of fact."

The language of the Ford Foundation Report with respect to its model is revealing. "An economic model developed for the project by Data Resources Incorporated provides a broad-based measure of the impact of reduced energy growth and concludes that a transition to a slower growth--even zero energy growth--can indeed be accomplished without major economic cost or upheaval. The study indicates that it is economically efficient as well as technically possible over the next 25 years to cut rates of energy growth at least in half. Energy consumption levels would be 40 to 50 percent lower than continued historical growth rates would produce at a very moderate cost of GNP--scarcely 4 percent below the cumulative total under historial growth in the year 2000, but still more than twice the level of 1975." No qualifying statements are made.[2]

First, as all of us here are painfully aware, the degree of accuracy of all quantitative models of the economy is questionable, especially when they are used for projecting for long periods into the future. The idea that they could identify a 4 percent difference in cumulative GNP over many years is incredible. If there are not problems with the structure of the model, there are data problems. For example, the parameters of the model used in the Ford Foundation study were estimated from data from the period covering 1950 to 1970. In many respects we have moved entirely outside the range of variation covered during that period, especially in the areas pertinent to the model, such as fuel prices, domestic energy sources, and international trade conditions.

Second, one may have questions about the specific structure of the model. It is, for example, highly aggregated; it contains only nine sectors of which five are energy sectors. Is it really possible to address the problem at hand with so few production sectors? Moreover, it appears that the basic structure of the model will predetermine one of the main results that it is said to have found, i.e., that energy usage does not have much to do with economic growth. The relationship between energy input and economic output and energy cost is based on the assumption that the increasing use of energy per unit output during the period when energy costs were falling can be extrapolated to a future situation in which energy costs rise. That is, the energy output relationship is reversible given a reversal of the historical trend in real prices. Aside from the question of whether dynamics of the real economic system permit such reversibility, there is the question of relationships between energy input and man-hour productivity. One may reasonably hypothesize that one factor in the increase in man-hour productivity in the post-war period is the substitution of inanimate energy for human energy. If this substitution effect is important, then a reversal of the situation would surely result in a reduction in productivity and a slower rate of economic growth. In the model, however, the factors determining aggregate output appear to be entirely uncoupled from any relations of this sort. Productivity is exogenously given. Should we then be surprised that the cost and rate of growth of energy use do not much affect the rate of GNP growth? That they do not is one of the principal conclusions of the study, but whether it is a conclusion or whether it is built into the assumptions of the model is questionable.

This problem concerning the appropriateness of asking models to answer policy-type questions is unanswered. It may be wise, at least when such models are used by public agencies and particularly Federal agencies, to create a model review board. Its duty would be to assess and pass judgment on the suitability of various models to address agencies' problems.

Models of Economic Environmental Systems

To try to understand the results of policy actions, different institutional structures for decisionmaking, alternative technologies, etc., a number of models of economic-ecological systems have been built. Since these are of more direct interest to our session than the energy model discussed in the last section, a few generalizations about this type of modeling would be useful before moving on to a specific application.

It is often said that the first principle of ecology is that everything is connected to everything else. This is perhaps true but somewhat unhelpful; however, it does bring into focus the question of how far modelers should go in the explicit incorporation of interdependencies. This is a general problem in systems analysis but it takes on additional force in connection with environmental problems because of the prominence of "ecological thinking" in the field. The "frog in the hole in the bottom of the sea" chain of reasoning of some ecologists has led to visions of the environmental management problem which push it beyond the bounds of successful modeling. Years ago, when operations research was first being explored by economists, Robert Dorfman wrote a fine article stating the general point very well.[3] In it, he said:

"As a result of complexity the operations analyst, like every other worker, lives always near the end of his tether. He simplifies his problem as much as he dares (somewhat more than he should dare), applies the most powerful analytical tools at his command, and with luck just squeaks through. But if all established methods fail, either because the problem cannot be forced into one of the standard types or because after all acceptable simplifications it is still so large or complicated, the equations describing it cannot be solved. When he finds himself in this fix, the operations analyst falls back on simulation or gaming."

One result of the ability of simulation to treat relationships beyond those manageable in optimization problems is that much discipline and order is lost, and the problem of choosing among alternative outcomes of the simulation can easily become impossible.

Consider a small simulation model in which there are 28 variables (an actual environmental model may easily have many hundreds), each of which may be set at any one of three levels. There are then 3^{28} possible designs of the system. This is approximately 23 thousand billion. If it takes 2 minutes of computer time to simulate each design, about 100 million years could be required to complete the simulation. Of course no simulator would attempt the complete enumeration of outcomes in a large problem, but this calculation does suggest the complexities involved. This and the paucity of data available for defining relationships specifying coefficients have been among the problems which doomed some of the more ambitious ecological modeling efforts to costly failure.

The elementary set of needs in economic-ecological modeling is that (1) the model must be persuasive, i.e., it must represent something in the real world with sufficient fidelity that a decisionmaker could with some confidence base a decision on it and (2) that some reasonably straightforward and efficient criteria must exist for choosing among vast numbers of alternative results.

Of course simulations can be very useful if informed judgment readily yields a few alternative systems for analysis. But it seems this is an unusual situation when large environmental systems are at issue. Simulation models can also be supplied with objective functions and one or another form of sampling can be used to generate a "response surface." The principles of sampling for this kind of problem are not well understood, however, and providing an adequate sample may be an extremely large problem in itself if the number of variables and alternative scales is great and the response surface is irregular. Otherwise, the process may come to a halt at the top of a gentle rise while totally ignoring the neighboring mountain peak.

Perhaps it is essential that we accept some form of optimization models, with all their limitations, as the only ones likely to be useful for decisionmaking in large problems like environmental management--although our experience is not so extensive that this conclusion can be drawn with certainty. Optimization models can, of course, incorporate simulation submodels to provide descriptive linkages in a set of nested models. But they do not sacrifice specifying a criterion function and require an orderly approach to the optimal solution. Selected parameters of the optimization model can be varied and new solutions found. This would almost always be desirable in any real decision situation. The device of an objective function with constraints and a specific solution procedure is not abandoned, however.

Clearly it is necessary to recognize that these models can never be "comprehensive" in the sense that they consider all linkages and all alternatives. Great care must therefore be taken to specify what aspects of reality are and are not included. In this connection, a well functioning market system can be of great help, which is often ignored in the more ecologically oriented models. We may exclude many aspects of resource use from explicit consideration in our environmental policy or management models on the grounds that they are appropriately handled by the market exchange system. The interface between these processes and the model as such is through the system of values generated by the market, that is, prices. The model itself can then focus explicitly on those aspects of resource use where the market exchange is known to fail seriously as an allocative device, e.g., with respect to allocating common-property environmental resources of air, water, and associated ecological systems.

Static and dynamic elements are likely to be particularly difficult to handle adequately in optimization models, and these are important deficiencies. Sensitivity analysis and the like can help, but the wise modeler will never let himself think that his models will provide a complete basis for decisionmaking either on conceptual or empirical grounds in a field as complex as environmental quality. Models must be viewed as potentially helpful tools which constitute an element, albeit a major one, in the decisionmaking process. They are tools which can reveal obscure impacts of common-sense policies and quantify them to some extent. They must be built and used because of the inherent logic demands of the problem and because we have nothing better.

The Regional Residual Model

I would like to conclude this introductory paper by discussing in general terms an environmental modeling enterprise which took place in the Quality of the Environment program at Resources for the Future while I was program director. The specific form and structure of the model was very much a result of the preceding type of consideration. It was developed by a team of researchers representing several disciplines and is often called the Russell-Spofford model, or more fully, the Regional Residuals Management model. It is a static optimization type model built for application to the Delaware Estuary Region for several purposes. For example, it could help test the impact on the cost of environmental management of introducing exotic technologies, such as stream reaeration, into the system. It could play out economic, in the sense of efficiency and distributional, implications of setting ambient standards at various levels in the region. In a politicized version it was useful in testing certain hypotheses on how the structure of legislative processes would affect decisions on environmental quality, e.g., referenda versus COGS versus small district representation in legislative assemblies. (For a relatively full report, see Reference 4.)

Here I wish only to say something about the structure of the model and particularly the light it sheds on one of the main hypotheses we sought to test with it--that there are important nonmarket linkages among the environmental media of land, water, and air, and that treating each in isolation as is done in current legislation and administrative practice is likely to lead to unanticipated and probably inefficient results. This is what might be called the basic EPA hypothesis.

The Russell-Spofford Model*

The Russell-Spofford model is, as already implied, designed to deal simultaneously with the three major general types of residuals--airborne, waterborne, and solid--and reflects the physical links among them in a regional context. It "recognizes," for example, that the decision to remove waterborne organic wastes by standard sewage treatment processes creates a sludge which, in turn, represents a solid residuals problem; the sludge must either be disposed of on land or burned, the latter alternative creating airborne particulates and gaseous residuals.

The model also can incorporate the nontreatment alternatives available (especially to industrial firms) for reducing the level of residuals generation. These include: input substitution (as natural gas for coal); change in basic production methods (as in the conversion of beet sugar refineries from the batch to continuous-diffusion process); recirculation of residual-bearing streams (as in recirculation of condenser cooling water in thermal-electric generating plants); and materials recovery (as in the recovery and reuse of fiber, clay, and titanium from the "white water" of papermaking machines). These alternatives are included by means of industrial linear programming submodels.

The model uses environmental diffusion models but it is also capable of incorporating environmental simulation submodels. In practice, the latter takes the form of an aquatic ecosystem model which translates residuals discharges into impacts upon various species of concern to man.

In addition to these features, the model incorporates a unique political (collective choice) feature. I think it is fair to say that this model is at the frontier of quantitative research in environmental economics.

The model containing these features is shown schematically in Figure 1. The three main components of the overall framework may be described as follows:

A Linear Programming Model. This model relates inputs and outputs of selected production processes and consumption activities at specified locations within a region, including: the unit amounts and types of residuals generated by the production of each product, the costs of transforming these residuals from one form to another (gaseous to liquid in the scrubbing of stack gases), the costs of transporting the residuals from one place to another, and the cost of any final discharge-related activity such as several types of landfill operations.

The programming model, which actually consists of an array of submodels pertaining to individual industrial plants, landfill operations, incinerators, and sewage treatment plants, permits a wide range of choices among production processes, raw material input mixes, by-product production, materials recovery, and in-plant adjustments and improvement. All these choices can reduce the total quantity of residuals to be disposed of. That is, the residuals generated are not assumed fixed either in form or in quantity. This model also allows for choices among treatment processes and hence among the possible forms of the residual to be disposed of in the natural environment and, to a limited extent, among the locations at which discharge is accomplished.

Environmental Models-Physical, Chemical and Biological. These component models describe the fate of various residuals after their discharge into the natural environment. Essentially, they may be thought of as transformation functions operating on the vector of residuals discharges and yielding another vector of ambient concentrations at specific locations throughout the environment (these are the now familiar diffusion models) and, in some instances, impacts on living things (these are aquatic ecosystem models reaching beyond the Streeter Phelps formulation). In aquatic ecosystem models, living creatures which participate in these processes are explicitly included in the model and the output is stated in terms of impact on living things (e.g., plankton and fish) rather than on physical parameters such as dissolved oxygen.

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*This portion of the paper is based largely on material prepared by my former associates at RfF, Clifford Russell and Walter Spofford.

A Set of Receptor-Damage Functions. These functions relate the concentration of residuals in the environment and the impact on living things to the resulting damages, whether these are sustained directly by humans or indirectly through impacts on material objects or on such receptors as plants or animals in which man has a commercial, scientific, or aesthetic interest. Ideally, for a full-scale overall efficiency version of the model, the functions relating concentrations and impacts on species to damage should be in monetary terms. In fact, the model as finally implemented is designed to meet environmental standards. However, its solution technique is based upon "penalty functions" and, therefore, proceeds as though violations of the standards carried a price. Since the objective is to meet environmental standards the price of violation is set very high.

The linkage between the components of the model and the method of optimum seeking may be illustrated as follows: Solve the linear programming model initially with no restrictions or prices on the discharge of residuals. Using the resulting initial set of discharges as inputs to the models of the natural environment, and the resulting ambient concentrations and impacts on living things as the arguments of the penalty functions, the marginal penalties can be determined as the change in penalties associated with a unit change in a specific discharge. These marginal penalties may then be applied as interim effluent charges on the discharge activities in the linear model, and that model solved again for a new set of production, consumption, treatment, and discharge activities. With appropriate bounds constraining consecutive solutions, the procedure is repeated until a position close to the optimum is found. This process can be looked upon as a steepest ascent technique for solving a nonlinear programming problem.

The Russell-Spofford model was designed for the analysis of residuals management in regions where the scale and severity of the problems justify a considerable investment in data and analysis. The model is still in the process of being applied to the Delaware Valley, which is discussed in the next section.

The Lower Delaware Valley Region

The Lower Delaware Valley region, chosen for this application, is a complex region with many individual point and nonpoint sources of residuals discharges. It is defined by county boundaries, shown in Figure 2. The grid superimposed on the figure is used for locating air pollution sources and receptors in the model. It is related to the Universal Mercator grid.

The region consists of Bucks, Montgomery, Chester, Delaware, and Philadelphia counties in Pennsylvania; Mercer, Burlington, Camden, Gloucester, and Salem counties in New Jersey; and New Castle County in Delaware. The major cities in the area are Philadelphia (coterminous with Philadelphia County); Trenton in Mercer County; Camden in Camden County; and Wilmington in New Castle County. Overall, the population of the area in 1970 was a little more than 5.5 million. Of this, 35 percent is accounted for by Philadelphia alone, with a further 5 percent found in Trenton, Camden, and Wilmington. However, other parts of the region are also heavily urbanized.

The region as a whole contains an abundance of manufacturing plants. In fact, it is one of the most heavily industrialized areas in the United States. It has, for example, 7 major oil refineries, 5 steel plants, 16 major pulp and paper or paper mills, 15 important thermal power generating facilities, numerous large and small chemical and petrochemical plants, foundaries, and large assembly plants for the auto and electronic industries. This, of course, made the task of identifying sources of residuals discharges, estimating the costs of discharge reduction for them, and including them in the regional model an enormous one. The model used contains 125 industrial plants, 44 municipal sewage treatment plants, and 23 municipal incinerators, which are all dealt with as point sources. In addition, there are 57 home and commercial heating sources with controllable discharges, each of which is treated as an area source, i.e., not tied to a specific stack location. Other point and nonpoint sources distinguished in the region are incorporated as background discharges.

The large population of the region naturally produces vast quantities of residuals from consumption activities requiring correspondingly large facilities for their handling and disposal. There are 7 municipal sewage treatment plants with flows greater than 10 million gallons per day (mgd) and 17 with flows greater than 1 mgd, counting only those discharging directly to the Delaware Estuary. On the major tributaries to the estuary and the Schuylkill River, there are more than 120 municipal treatment plants of widely varying sizes. For the disposal of solid residuals there are 17 incinerators currently operating with an aggregate capacity of about 6,000 tons per day, and many major and minor landfill operations. Together, on an annual basis, the heating of homes and commercial buildings is responsible for about one-quarter of the total discharges of SO_2 and 10 to 15 percent of the particulate discharges in the region.

The major recipient of waterborne residuals in this area is the Delaware Estuary itself. The Estuary is generally taken to be the stretch of river between the head of the tide at Trenton and the head of the Delaware Bay at Liston Point, Delaware. For analysis purposes the estuary was divided into the same 22 reaches shown in Figure 3.

The low flow of the river varies widely from month to month and year to year. For aquatic ecosystem modeling purposes, a relatively low flow period was selected.

For the modeling of air quality, the atmospheric conditions used represent the annual joint probability distribution of wind speed, wind direction, and stability conditions for 1968, assumed uniform throughout the region. Conditions representing rare events were not used in the model for either air or water quality analyses. Ideally, explicit attention would also be given to this aspect of the modeling, but mathematical programming models do not lend themselves well to the ideal analysis of systems in which random events occur. As I mentioned earlier, this is one of their weaknesses.

Contents of the Model

The model framework was discussed in general terms earlier in this paper in connection with Figure 1. Here the discussion is more detailed in order to grasp the nature of the actual application of the concepts outlined there. The model is designed to provide the minimum-cost method of simultaneously meeting several sets of exogenously determined standards. Two of them are of interest here.

Minimum Production Requirements. This means bills of goods for the individual industrial plants, heat requirements for home and commercial space heating, and specified quantities of liquid and solid residuals requiring some disposal action by municipalities.

Levels of Ambient Environmental Quality. This is represented, for example, by maximum concentrations of SO_2 and suspended particulates at a number of receptor locations in the region, minimum concentrations of dissolved oxygen and fish biomass in the estuary, maximum concentrations of algae in the estuary, and restrictions on the types of landfill operations which can be used in the region.

In Figure 4, more detail is given on how the model functions. In the upper left of the diagram is found the basic driving force for the entire model, the linear programming model of residuals generation and discharge. It is in this part of the model that minimum "production" constraints are found. A key output of this part, as mentioned in connection with Figure 1, is a vector of residuals discharges, identified by substance and location. These discharges feed into the environmental models--the model of the aquatic ecosystem and the dispersion model for the suspended particulates and SO_2 discharges. This section of the overall model, in turn, produces as output a vector of ambient environmental quality levels (for example, SO_2 concentrations) at numerous designated points in the region. These concentrations are then treated as input to the "evaluation" submodel found in the lower right of the diagram. Here the concentrations implied by one solution of the production submodel are compared with the constraints imposed for the model run, and the penaty function procedure is used to iterate the model until all constraints are met, within some specified tolerance.

The Production Model

In fact, as was also indicated in connection with Figure 1, the production model consists of a number of sets of linear programs with each set arranged in a module. The modules reflect the chronological development of the model as it was expanded over time to encompass more and more of the activities in the region. A summary of this part of the model is shown in Table 1. The modules are shown in the first column. The designation MPSX derives from the particular computational routine used in the analysis. The next three columns give the dimensions of the LP matrix for each module and the number of discharges. Residuals generated by the linear programs for these activities reflect operating conditions as of about 1970, and represent generation under steady-state conditions. Variability of residuals generation in the various activities was not considered. It will be noted that the overall program has over 3,000 rows and nearly 8,000 columns. Included are 306 sources of discharges, with options for reducing discharges. For the number of discharges and types of residuals being considered, there are nearly 800 specified residuals being discharged to the various environmental media. The next column gives the type of activities in each module.

Only the powerful capacity of contemporary computing machines makes it feasible to solve a problem of this size. Even so, scaling down the model to fit the capability of even a large computer was a difficult practical problem.

The Environmental Models

The overall model incorporates a 22-reach nonlinear ecosystem model of the Delaware Estuary. Inputs of liquid residuals discharges to this model include: organics (BOD), nitrogen, phosphorus, toxics, suspended solids, and heat (Btu). Outputs are expressed in terms of ambient concentrations of algae, bacteria, zooplankton, fish, oxygen, BOD, nitrogen, phosphorus, toxics, suspended solids, and temperature. Three of these outputs--algae, fish, and oxygen--are constrained (all can be constrained in the model). In addition, the model includes two 57 x 251 (57 receptor locations and 251 dischargers) air dispersion matrices, one for sulfur dioxide and one for suspended particulates. These relate ambient ground-level concentrations to residuals discharges (SO_2 and particulates).

Results

At the time of this writing, production runs with the large model have just gotten underway. A few preliminary results, however, can be presented with respect to the "EPA hypothesis."

First, the model shows that in this realistic setting of an actual case there are significant linkages among the management aspects of the different residuals types. Tighter ambient standards for the atmosphere do significantly affect the cost of maintaining water quality standards and vice versa. This can be seen by considering the following example results from production runs with the model.

Air

	Easy ambient standards	**Tight ambient standards**
Easy ambient standards	$395,640	1,064,892
Water	↓Δ = $26,391	↓Δ = $244,379
Tight ambient standards	$422,031	1,309,271

High quality landfill required for all runs.

All the numbers in the table refer to total additional costs to the region for meeting environmental standards in dollars per day. The sample runs show that going from easy (relatively low) water standards to tight (relatively high) water standards costs about $26,000 per day when only easy air standards are imposed. If, however, tight air standards are required, going from easy to tight water standards costs about $244,000, or almost ten times as much. Thus, the model tends to support the EPA hypothesis that, taken in a realistic regional context, there are linkages among the different environmental media in the realistic setting of an important region and that they are of substantial magnitude. Policymaking, planning, and administration which ignore them are likely to encounter untoward surprises.

Perhaps even more important, the Delaware application indicates that it is possible to develop an integrated residuals management model for a large region at a manageable cost. The cost of this model (granted that much of the basic data had been collected already) was about 10 man-years of effort on the part of the senior researchers, some research assistance, and perhaps $100,000 worth of computer time at commercial rates. In dollars, the cost could be put at roundly $1 million, or about 1 day's worth extra cost to the region of operating with tight environmental standards.

Conclusion

In conclusion, it seems appropriate to return to the question of the choice of models. Mathematical models for analysis of environmental and other resources problems must be designed for specific purposes if they are to be useful. There is no such thing as a general model. If models are regional in character, it is usually even difficult to transfer them to another region. Such models must not be asked questions they were not designed to answer. This seems obvious but there are important instances in which this is happening.

On the matter of optimization versus simulation models, the question may be discussed by summarizing the considerations which enter into the choice in relation to residuals-management-type models. It should be remembered that, as illustrated by the Russell-Spofford model, combinations of simulation and optimization are possible.

1. Mathematical optimization imposes a valuable discipline on the modeler and the modeling process.

2. If ambient standards are the targets to be achieved by a control strategy and there are a large number of dischargers, a large number of receptors, and a large number of possible discharge reduction options, mathematical optimization is usually the reasonable way to proceed.

3. If there are only a few major dischargers and a few options for reducing residuals discharges, simulation may be easier and sufficiently efficient.

4. If there are many similar sources of residual discharges, but only one or two options for reducing discharges at each source, and the objective is defined in terms of required reductions or percent reduction at the sources rather than in terms of ambient conditions, simulation again may be easier and sufficently efficient.

5. Large mathematical optimization models are expensive and difficult, unless they are linear.

6. Large, nonlinear mathematical optimization models frequently have multiple "optima" and it is usually difficult to identify and deal with this situation when it exists.

7. The linearity assumptions may or may not do great violence to the real world.

8. Synergistic and antagonistic effects are more difficult to handle in mathematical optimization than in simulation models.

9. Economies of scale or analogous increasing-return situations cannot be handled satisfactorily by any mathematical optimization technique.

10. Time-dependent phenomena are difficult to handle in optimization models.

The balance of these considerations will usually point to optimization as the preferred approach of the problem is large and complex.

Finally, it should be remembered that any approach to analyzing a complex environmental management problem involves obtaining, arranging, and handling large amounts of empirical data. In many cases the major problem is that of obtaining empirical data on activities--production process, residuals generation, and residuals discharge reduction options and their costs--and on the effects of discharges on ambient conditions.

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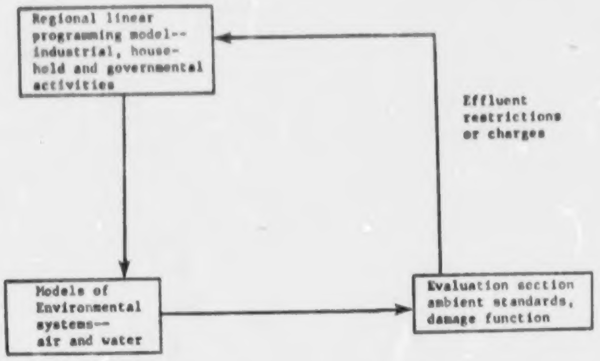
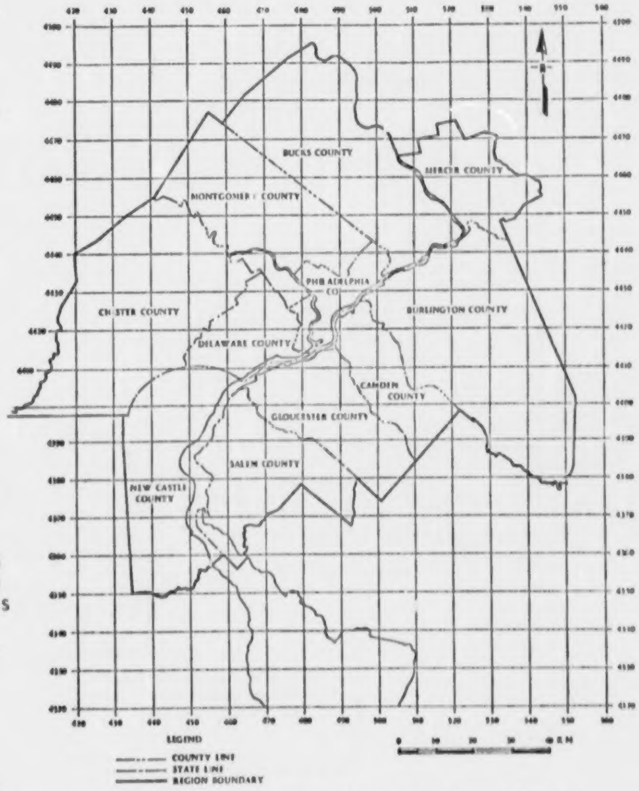

Regional linear programming model--industrial, household and governmental activities
Effluent restrictions or charges
Models of Environmental systems--air and water
Evaluation section ambient standards, damage function

Figure 1. Schematic of Regional Residuals Management Model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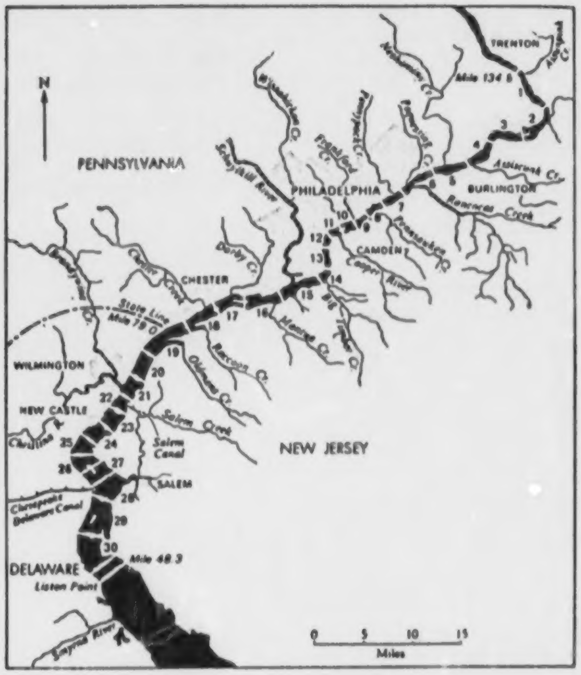
CAMDEN COUNTY
GLOUCESTER COUNTY
SALEM COUNTY
NEW CASTLE COUNTY
LEGEND
COUNTY LINE
STATE LINE
REGION BOUNDARY

Note: The grid is in kilometers and is based on the Universal Transverse Mercator (UTM) grid system.

Figure 2. Lower Delaware Valley Region


N
TRENTON
Mile 134.5
PENNSYLVANIA
PHILADELPHIA
BURLINGTON
Schuylkill River
Frankford Cr.
Assiscunk Cr.
Rancocas Creek
Pennsauken Cr.
CAMDEN
Cooper River
CHESTER
Chester Creek
Darby Cr.
Brandywine Cr.
State Line
Mile 78.0
Big Timber Cr.
Mantua Cr.
Raccoon Cr.
Oldmans Cr.
WILMINGTON
NEW CASTLE
Christina R.
Salem Creek
Salem Canal
SALEM
NEW JERSEY
Chesapeake Delaware Canal
DELAWARE
Liston Point
Mile 48.3
Smyrna River
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
0
5
10
15
Miles

Source: FWPCA, *Delaware Estuary Comprehensive Study.*

Figure 3. Map of the Delaware Estuary Showing Analysis Sections

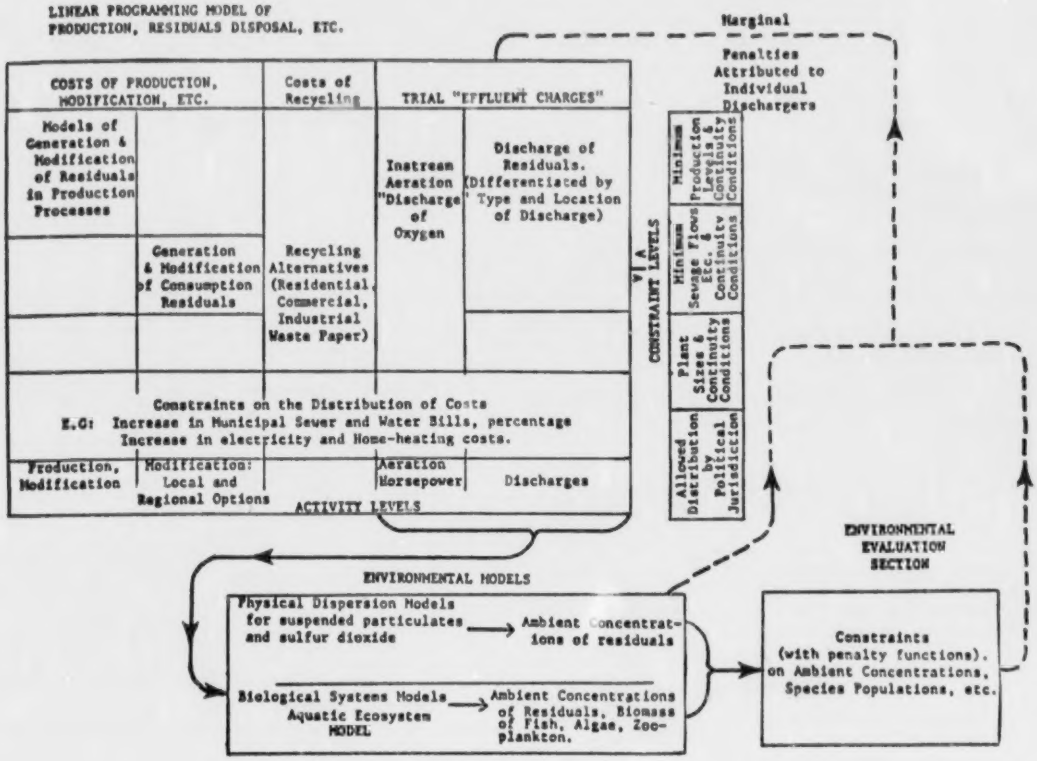

LINEAR PROGRAMMING MODEL OF PRODUCTION, RESIDUALS DISPOSAL, ETC.
COSTS OF PRODUCTION, MODIFICATION, ETC.
Costs of Recycling
TRIAL "EFFLUENT CHARGES"
Models of Generation & Modification of Residuals in Production Processes
Generation & Modification of Consumption Residuals
Recycling Alternatives (Residential, Commercial, Industrial Waste Paper)
Instream Aeration "Discharge" of Oxygen
Discharge of Residuals. (Differentiated by Type and Location of Discharge)
Constraints on the Distribution of Costs
E.G: Increase in Municipal Sewer and Water Bills, percentage Increase in electricity and Home-heating costs.
Production, Modification
Modification: Local and Regional Options
Aeration Horsepower
Discharges
ACTIVITY LEVELS
≤ ≥
CONSTRAINT LEVELS
Minimum Production Levels & Continuity Conditions
Minimum Sewage Flows Etc. & Continuity Conditions
Plant Sizes & Continuity Conditions
Allowed Distribution by Political Jurisdiction
Marginal
Penalties Attributed to Individual Dischargers
ENVIRONMENTAL MODELS
Physical Dispersion Models for suspended particulates and sulfur dioxide
Ambient Concentrations of residuals
Biological Systems Models Aquatic Ecosystem MODEL
Ambient Concentrations of Residuals, Biomass of Fish, Algae, Zooplankton.
ENVIRONMENTAL EVALUATION SECTION
Constraints (with penalty functions). on Ambient Concentrations, Species Populations, etc.

Figure 4. Schematic Diagram of the Regional Residuals Management Model

Table 1. Delaware Valley Model

Residuals Generation and Discharge Modules

Module Identification	Size of Linear Program			Description	Extra Cost Constraints
	Rows	Columns	Discharges		
MPSX 1	286	1649	130	Petroleum Refineries (7) Steel Mills (5) Power Plants (17)	57 Electricity (percent extra cost)
MPSX 2	741	1474	114	Home Heat (57)	57 fuel (percent extra cost)
				Commercial heat (57)	57 fuel (percent extra cost)
MPSX 3	564	1854	157	"Over 25 μgms/m^3" dischargers (75)	
MPSX 4	468	570	180	Delaware Estuary Sewage Treatment plants (36)	36 sewage disposal ($ per household per year)
MPSX 5	923	1778	86	Paper plants (10)	
				Municipal Incinerators (23)	
				Municipal solid residuals handling and disposal activities	57 solid residuals disposal (percent extra cost)
MPSX 6	228	394	116	Delaware Estuary industrial dischargers (22)*	
				Instream aeration (22)	57 instream aeration (absolute extra cost)
Total	3210	7719	783		

* Twelve of the Delaware Estuary Industrial Wastewater discharges in MPSX 6 are also represented by SO_2 and/or particulate discharges in MPSX 3.

ECONOMIC IMPLICATIONS OF POLLUTION-INTENSIVE EXPORTS BY DEVELOPING COUNTRIES

Peter A. Petri
Department of Economics
Brandeis University
Waltham, Massachusetts

SUMMARY

A new, detailed world model is described and used to identify some economic implications of exports of pollution-intensive products by so-called "fourth world" countries. For these nations, pollution-intensive exports are found to be unattractive relative to conventional types of exports from the viewpoint of various economic criteria. Still, pollution-intensive exports are found to generate net earnings of foreign exchange, a factor critical to the development prospects of resource-poor, low-income regions.

1. Introduction

At the request of the United Nations, a team of economists at Brandeis and Harvard Universities has recently assembled a comprehensive, disaggregated, multi-regional model of the world economy.[1] The purpose of the model is to shed light on the alternative paths the world economy could follow over the next three decades. To this end, the model contains a large amount of detailed information on natural resources, agriculture, industry, and the environment. It is used here to assess the economic consequences of certain alternative export strategies for a group of developing nations.

In a series of projections described elsewhere,[2] the model has shown that the attainment of reasonable growth targets for a large part of the developing world will require substantial improvements in their export capabilities. If the export positions of these nations were to evolve along historically established trends, the sharp disparities in income that now prevail would widen in the future. The prospects for developing countries without substantial resource endowments (the so-called "fourth world") are especially vulnerable to the projected external payments imbalances. These problems motivate the search for alternative export strategies for these nations—including two particular approaches investigated in this paper.

The first of these strategies would involve stepped-up exports of commodities that are conventionally thought to represent the comparative advantages of a developing economy. The second strategy would focus on exports of products manufactured by relatively pollution-intensive processes. This latter approach rests on the assumption that the absorptive capacities of the environment are greater in areas that have not yet experienced extensive industrialization, and that this fact might obviate the need for costly abatement measures. It is not our purpose to test the validity of these assumptions. Rather, we concentrate on the purely economic (in contrast to environmental) implications of the two alternatives.

An important secondary objective of this paper is to provide a direct, though simple, example of how the new world model can be used to study questions in international policy. The next section offers a general overview of the model's structure, though obviously its precise technical details cannot be adequately described in so short an essay.[3]

2. The Model

The world model consists of 15 sub-models, each representing (in terms of some 175 equations and 229 variables) the economic structure of a particular region. The sub-models are linked by a network of trade, that is, by detailed inter-regional flows of goods, services, and various types of capital.

The parameters of the system, that is, the quantitative descriptions of the regional units, were first estimated for 1970, and then projected forward to 1980, 1990, and 2000. These four parallel systems, describing the state of the world economy at the end of each decade, are linked in turn by the growth (in the case of capital) and depletion (in the case of resources) of certain detailed stocks.

Figure 1 illustrates, albeit in highly simplified form, the critical interdependencies within a given regional sub-model. Figure 2 gives some indication of how the sub-models are linked. The system is in fact a good deal more flexible than Figure 1 indicates. New variables or equations can be readily added. Also, the direction of the logical flow can be changed by varying which variables are prespecified and which are endogenously determined in a given application. Figure 1 presents the basic specification used in the analyses of later sections; this structure reflects one of many possible specifications of the system.

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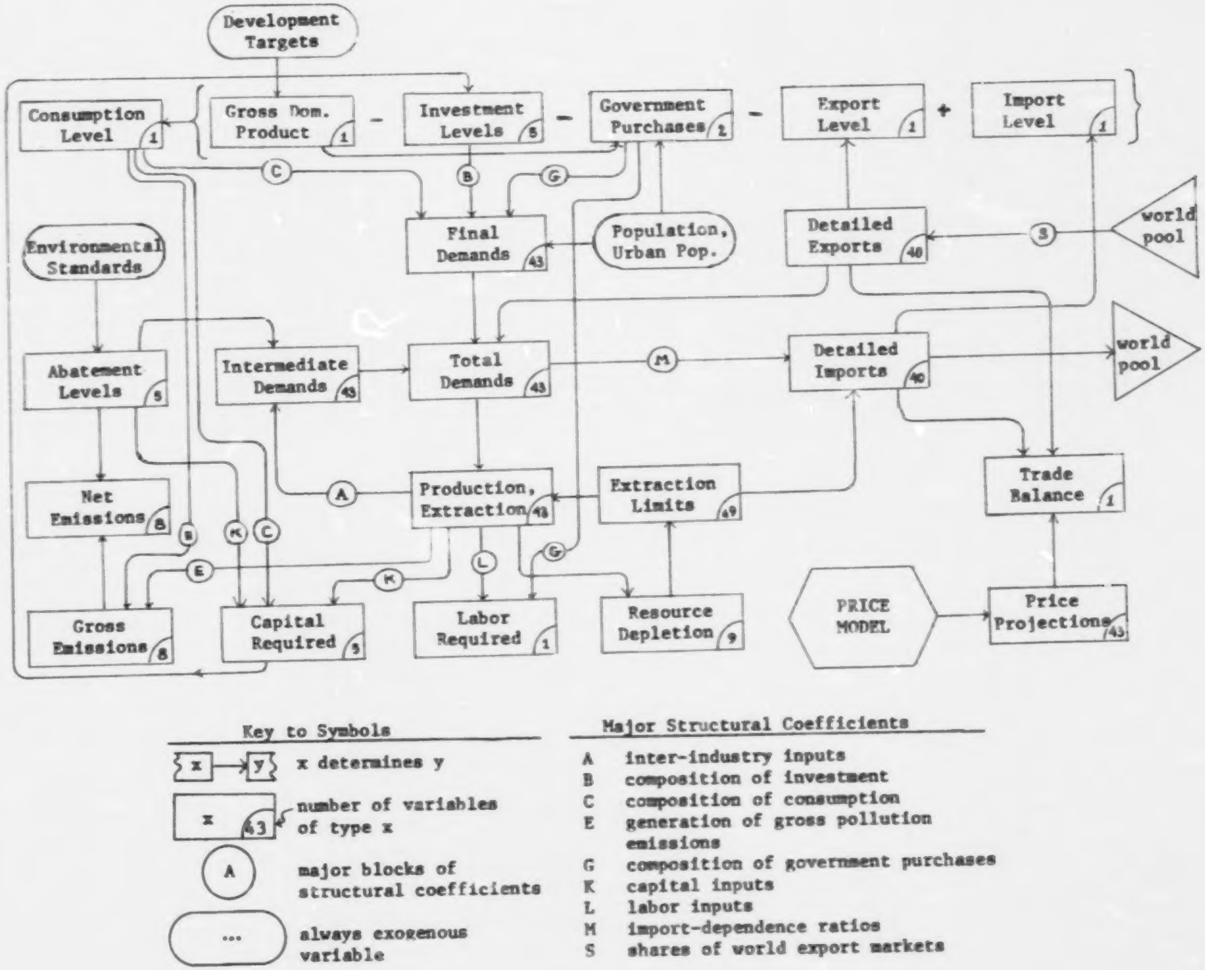
[1] Officially, this project was described as the "Study on the Impact of Prospective Environmental Issues and Policies on the International Development Strategy." The senior research team was headed by W. Leontief, and included A. P. Carter, J. J. Stern and the author. The model used in this paper is, of course, a joint product of the group; however, the other members of the team do not necessarily share the particular conclusions and views expressed here.

[2] P. A. Petri and A. P. Carter, "Resources, Environment, and the Balance of Payments: Application of a Model of the World Economy," delivered at the Third Reisenburg Symposium on the Stability of Contemporary Economic Systems, forthcoming in the Conference volume.

[3] Preliminary "Technical Report" prepared for CDPPP, United Nations, May 1975, describes the model more fully. A final version will be published by United Nations shortly.

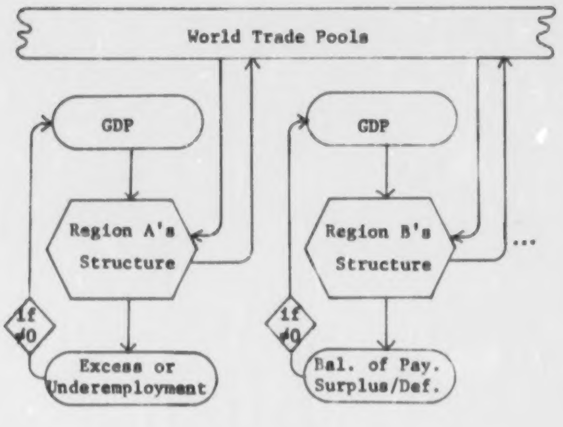
Figure 1. Internal Structure of a Region


Development Targets
Consumption Level 1
Gross Dom. Product 1
-
Investment Levels 5
-
Government Purchases 1
-
Export Level 1
+
Import Level 1
C
B
G
Environmental Standards
Final Demands 43
Population, Urban Pop.
Detailed Exports 40
S
world pool
Abatement Levels 5
Intermediate Demands 43
Total Demands 43
M
Detailed Imports 40
world pool
Net Emissions 8
B
K
C
A
Production, Extraction 43
Extraction Limits 49
Trade Balance 1
E
K
L
G
Gross Emissions 8
Capital Required 5
Labor Required 1
Resource Depletion 9
PRICE MODEL
Price Projections 43
Key to Symbols
x
y
x determines y
x
43
number of variables of type x
A
major blocks of structural coefficients
...
always exogenous variable
Major Structural Coefficients

A	inter-industry inputs
B	composition of investment
C	composition of consumption
E	generation of gross pollution emissions
G	composition of government purchases
K	capital inputs
L	labor inputs
M	import-dependence ratios
S	shares of world export markets

Figure 2

Interaction of Regions



The first full row of variables in Figure 1 shows how the overall level of consumption is determined. Here exogenous targets for gross domestic product (GDP) are given and the endogenously determined levels of investment, government expenditures, and foreign trade follow from them. The GDP targets in this case were supplied by the United Nations, and are consistent with the goals of the U.N.'s Second Development Decade. Government expenditures are determined partly by the GDP, and partly by the size of the urban population as it influences the requirements for urban services. Investment and import levels are determined by relationships further along the flowchart.

Exports are exogenous to a given region but endogenous to the world system as a whole. Figure 2 describes the trade model that links the 15 regional sub-models. The trade model leaves the determination of each region's imports to the structural equations describing that region. Import requirements are then summed across regions, and the resulting world demands are allocated to the regions as exports. The allocations are accomplished by export share coefficients specific to each traded commodity. These regional export shares, initially projected with regression studies based on historical and cross-section data, can be readily changed to accomodate alternative assumptions, as is done later in this paper.

Given the detailed list of exported commodities, and the levels of consumption, government expenditures and investment, it is now possible to specify the detailed final demands facing each regional economy. The transformations from overall demand levels to demands for specific commodities are accomplished by various converter coefficients representing the composition of consumption, investment, etc. These coefficients depend on the region's per-capita income, and also reflect, in some cases, region-specific influences on the commodity breakdown of demand. The detailed final demands are added to intermediate demands (the input requirements of producers) to arrive at the total domestic demands facing the regional economy.

Unlike most input-output based models, the system treats several key commodities and activities in their natural physical dimensions. Five agricultural commodities, nine exhaustible resource commodities, as well as eight pollutants are measured in metric tons or other relevant physical units. This feature makes it possible to use physical quantity data and to check the results against other detailed projections.

Domestic demands can be satisfied either by imports or by local production. Depending on the commodity, two different approaches are used to effect these allocations. In the case of exhaustible resource commodities, importing regions are assigned output levels consistent with the amount of regional resource reserves still available, and imports are used to fill all remaining unsatisfied demands. In the case of manufactured products, import dependency ratios are specified using, once again, regressions based on historical and cross-section data. These regressions indicate that a region's import coefficients generally vary inversely with economic size, and depending on the commodity, either increase or decrease as a function of the region's development level relative to the development levels of its foreign competitors. With one or the other of these approaches, the domestic demand for each commodity was apportioned between imports and domestic production.

In turn, the domestic output levels determine the demand for intermediate inputs and the requirements of various types of capital and labor. These requirements are calculated using input-output coefficients that vary with the region's development level, with time, and in some instances, with certain region-specific conditions.

The capital requirements of producers, along with the capital requirements of households and of the abatement activities are next used to determine the economy-wide level of total investment. These computations begin with the capital stocks available at the beginning of each decade, and arrive at the investment levels that provide for the replacement of worn-out plant and equipment and for the required net expansion of capacity.

As shown on the left side of Figure 1, production also results in "gross emissions" of various specific pollutants. A set of abatement activities, e.g., various levels of waste-water treatment, is specified as a means of controlling the pollutants generated in production and by households. Untreated emissions plus the residuals emitted by the abatement processes are summed to show the net emissions released into the environment. The usefulness of this information is limited, of course, by the present inability of the model to determine specific local concentrations within its large geographical areas.

On the right side of Figure 1, the detailed export and import levels are valued at projected prices in order to arrive at projected trade balances. The price model is independent of the physical system discussed so far, though it is based on many of the same assumptions, relationships, and structural coefficients.

The price model relies on the inter-industry structure of an advanced developed economy to examine the price implications of the various projected changes in the structural coefficients. The prices obtained are normalized to keep the value of a bundle of consumption goods constant throughout the projection period, and should therefore be interpreted as relative rather than absolute price projections.

The inputs structures of the resource industries played an important role in the estimation of future prices. As each region exhausted its high-grade reserves of a specific resource it was assumed to move to lower quality deposits. This meant, in turn, that extraction would entail higher input requirements (per unit of usable resource output) and hence higher costs. Specific (though obviously tentative) data about the quantity and quality of deposits in each region were used to trigger the changes in extraction input requirements. Of the relative price changes projected, a large part can be traced to the successive exhaustion of high-grade reserves of a number of resource commodities. Other, smaller effects arise because labor productivities are projected to grow at unequal rates in different sectors, and because various kinds of input substitution are expected to take place.

Our description has, so far, dealt with a particular structural specification based on exogenous GDP targets. Alternative specifications make it possible to ask rather different types of questions. For example, it might be useful to know what GDP levels might be attained given, say, limits on the available labor force. Figure 2 shows a schematic approach that assigns a unique specification to each regional sub-model, depending on the particular factors that are expected to govern that region's future development. In Region A, the supply of labor is assumed to limit the level of GDP. Conceptually, the appropriate level of GDP could be found by trial-and-error, as the level that (through the interactions described in Figure 1) results in "correct" labor requirements. In the case of Region B, balanced (or appropriately imbalanced) trade might be viewed as the relevant target. The computations do not in fact need to depend on a trial-and-error procedure: the results of the new specification can be obtained directly by modifying and solving the original simultaneous equation system used to describe the region.

A further implication of this approach is that several different instruments could be used to achieve the same ultimate outcome for any given target variable. In order to obtain balanced international accounts, for example, the region's share of world exports might be assumed to increase even though its GDP is held constant. Alternately, its import-dependency coefficients might be changed, or new assumptions might be introduced concerning international aid and capital flows.

3. The Experiment

The two hypothetical trade development programs (representing the conventional and pollution-intensive export strategies) will be examined in the context of the GDP-target specification shown in Figure 1. Earlier projections based on this structure have generally shown sizeable and deteriorating balance of payments deficits for developing regions without substantial resource endowments. These deficits are due to the rising prices of imported resource commodities, to the high import-intensity of capital formation in developing regions, and to the relatively slow growth of markets for the key exports of the developing world.

Against this background we turn now to examine the implications of a pollution-intensive export program for three developing regions: Latin America (Medium Income), Asia (Low Income), and Arid Africa.[*] It is clear, of course, that any strategy that results in a vigorous expansion of exports will also improve the exporter's balance of payments position. In order to identify the specific characteristics of the pollution-intensive program, we perform a controlled experiment; one that contrasts the effects of this strategy with the implications of more traditional approaches to export development.

In Experiment A, export increases are assumed to occur in five sectors (textiles and apparel, wood products, furniture and fixtures, printing, and miscellaneous manufactures) characterized by labor-intensive and relatively standardized production technologies. In Experiment B, the same amount of exports is assumed to be produced by a different group of sectors (primary metal processing, paper, industrial chemicals, rubber, and other chemicals), industries that are generally recognized as the most pollution-intensive among manufacturing processes.

Both programs are constructed to generate (by the year 2000) $50 billion of new exports for the three regions taken together. The $50 billion is divided among the regions in proportion to the currently projected exports. The increases are further assigned to specific products—within the industry group relevant to each experiment—in proportion to overall world trade in these products. The hypothetical export increases calculated this way are shown in Table 1.

Table 1. Alternative $50 bill. Export Strategies

($ bill., 2000 relative prices)

A. Conventional Exports[**]

	Latin America	Asia	Arid Africa
Textiles, Apparel	13.0	20.5	1.69
Wood Products	1.7	2.7	.23
Furniture, Fixtures	.3	.4	.03
Printing	1.2	1.8	.15
Miscellaneous Mfg.	2.3	3.6	.30
Totals (Σ = 50.0)	18.5	29.1	2.40

B. Pollution-Intensive Exports[**]

	Latin America	Asia	Arid Africa
Primary Metals	6.0	9.4	.78
Paper	4.0	6.3	.52
Rubber	1.0	1.6	.13
Ind'l Chemicals	4.4	7.0	.57
Other Chemicals	3.0	4.7	.39
Totals (Σ = 50.0)	18.5	29.1	2.40

[**] Detail may not add due to rounding.

The experiments were implemented by inflating each region's export share coefficients so as to generate the export increases of Table 1. Both programs are assumed to be phased in gradually over the 1970-2000 period, reaching the specified increases in the year 2000.

In the context of fixed GDP targets, the export increases have two immediate effects: first, exports displace consumption goods in production and, second, the export increases reduce the region's trade deficit. Secondary consequences follow from the fact that the input structures of the export-oriented sectors may be quite different from the input structures of the consumption-oriented activities that they replace. These precise consequences depend, of course, on the sectoral mix of the export program, and shall be examined shortly.

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[*] These three regions include (a) Argentina, Brazil, Mexico, Chile, Cuba; (b) Bangladesh, Pakistan, India, Indonesia; (c) Egypt, Ethiopia, Morocco, Sudan, plus in each case smaller countries.

While using the fixed-GDP specification, we shall not be able to measure directly the growth-generating consequences of either program. To do so, we would have to identify a specific limit on each region's development (as is done schematically in Figure 2) and experiment with the alternative export strategies under that particular constraint. To the extent that the programs affect the limiting factor differently, they would generate different rates of long-term growth.

At this stage, however, the fixed-GDP context offers a more general way of assessing the effects of each strategy on a set of different factors that potentially limit growth (including foreign exchange, capital, and labor)—without prejudging which of these factors is most acutely limiting. This is done in Section 4. The next logical step, the quantification of the ultimate development impacts of these effects, is left to future work.

4. Comparison of Alternative Export Strategies

Table 2 presents the balance of trade implications of the two strategies. In neither case is the net improvement (for the three regions taken together) as great as the $50 billion export increase; both export strategies involve leakages in the form of added import requirements. The import leakages of pollution-intensive exports are some $5.5 billion higher than those of the conventional strategy. Pollution-intensive industries tend to have above-average raw material and capital requirements, and these two kinds of commodities are heavily imported. In addition, the inter-industry purchases of pollution-intensive industries tend to favor the least developed and therefore most import-dependent sectors of a developing economy.

Table 2. Balance of Trade Results, 2000

A. Improvement of LDC Balances

($ bill., 2000 relative prices)

	Central Projection	Export Strategy A	Export Strategy B
Latin America	-84.6	-65.5	-69.1
Asia	-81.6	-58.8	-60.9
Arid Africa	- 7.9	- 6.4	- 6.2
Subtotal:	-174.1	-130.7	-136.2
Improvements over Central Projection:		+43.4	+37.9

B. Regional Distribution of the Losses Offsetting the LDC Improvements (percentages)

	Export Strategy A	Export Strategy B
Western Europe (High Income)	44	41
North America	9	27
Japan	16	9
Soviet Union	4	10
Eastern Europe	10	4
Western Europe (Medium)	6	1
Middle East	3	2
Asia, Centrally Planned	3	3
Latin America (Low Income)	1	1
Tropical Africa	1	1
Southern Africa	1	1
Total Losses	100%	100%
Total Losses in $	-43.4	-37.9

The rest of the world is differently affected by the two export alternatives. As the second part of Table 2 shows, the predominant effect of both strategies is to reduce the trade surpluses (or to increase the deficits) of advanced developed countries. The conventional exports are apparently diverted more sharply from Europe and Japan, while the pollution-intensive products are obtained more at the expense of North America and the Soviet Union.

The internal consequences of the trade alternatives are summarized in Table 3. The most striking differences emerge in the overall capital stock required in production. In Experiment A, the diversion of gross product from consumption-oriented activities to conventional exports has in fact saved capital inputs. In contrast, the pollution-intensive program imposes added capital requirements on the regional economy. While the $34.4 billion difference between the programs is small relative to the total capital stocks of the three economies, it is large when compared to the capital requirements of the programs themselves. It would take about 40% more capital to implement the pollution-intensive strategy than it would to produce equally valued conventional exports.

Table 3. Additional Requirements of Pollution-Intensive Strategy over the $50 bill. Conventional Strategy

($ bill., 1970 prices except as noted)

	All Three Developing Regions
Building & Plant Capital	18.1
Equipment Capital	16.3
Subtotal: All Fixed Capital	34.4
As % of Economy-wide Stock (%)	1.2
Annual Investment	2.3
Employment (mill. myr.)	1.5

The employment differences between the programs are small and mixed. Quite surprisingly, both programs tend to generate about the same amount of employment when all indirect effects are taken into account. Differences might be found if employment were further itemized by skill categories, but this refinement has not yet been implemented on the world system.

The environmental implications are shown in Table 4. While the economic differences between the alternative programs are found to be small relative to overall economic magnitudes, this is not the case with respect to the net emissions of specific pollutants. These added pollutant loadings are not easily interpreted in the absence of geographically detailed projections. Nevertheless, they suggest that a pollution-intensive export program that is large enough to affect the balance of trade will also have non-negligible environmental consequences.

If the difficulty of achieving one or the other of the export targets is related to the extent of the required structural transformation of the economy, our solutions can also shed light on the relative feasibility of the two programs. Table 5 shows the output changes implied by each of the programs relative to the standard projections for 2000.

The structural changes implied by the pollution-intensive alternative are typically larger than those for the conventional program, and especially so for the two poorest regions, Asia (Low Income) and Tropical Africa. This was to be expected, of course, since the conventional export bundle was designed to emphasize the strengths of a developing economy. The radically different output profiles obtained under Experiment B suggest that major changes would have to take place (in terms of new infra-structure, manpower training, and the establishment of supplying industries) before the new activities can be absorbed in the economic fabric.

Table 4. Additional Net Emissions with Pollution-Intensive Export Strategy, 2000

(percentages relative to projected emissions)

	Latin America	Asia	Arid Africa
Pesticides	-1	-2	-1
Particulates (Air)	68	11	9
BOD	12	5	3
Nitrogen (Water)	8	0	0
Suspended Solids	16	23	14
Dissolved Solids	8	8	3

Table 5. Additional Output Required to Implement Export Strategies in 2000

(percentages relative to projected output)

	Latin America	Asia	Arid Africa
A. Conventional Exports			
Textiles, Apparel	27	20	19
Wood Products	16	32	50
Furniture, Fixtures	-2*	-2*	0
Printing	8	37	40
Miscellaneous Mfg.	24	23	18
Five Industries Together	15	17	16
B. Pollution-Intensive Exports			
Primary Metals	19	67	42
Paper	26	75	40
Rubber	11	41	33
Ind'l Chemicals	20	35	17
Other Chemicals	17	33	30
Five Industries Together	22	49	30

* Since in our computation exports displace consumption in (fixed) GDP, and since furniture is important in consumption and not so in the export package, furniture output would decline if the strategy were implemented.

5. Conclusions

By postulating two hypothetical export programs, we have attempted to identify some economic consequences involved in the choice between conventional and pollution-intensive export strategies. The pollution-intensive approach is found to be more expensive in terms of capital, and requires more imports. Moreover, this approach would imply sizeable shifts in the output mix of the developing economy, and might create non-negligible environmental repercussions. Also, at least initially, the pollution-intensive sectors would tend to operate as an enclave within the regional economy.[4]

In sum, several economic criteria mitigate in favor of the conventional and against the pollution-intensive strategy—provided, and this is quite important, that a choice exists at all. Even the pollution-intensive approach, relying as it does on some resources that are especially scarce to a developing economy, does generate foreign exchange, and would, in the absence of other earning opportunities, most likely contribute to the development process.

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[4] Some dynamic theories of development suggest that the early establishment of basic industries—as the pollution-intensive sectors typically are—can actually hasten development through a variety of backward and forward linkages with other sectors of the economy. These effects would have to be large in order to offset the static disadvantages cited above.

A TAXONOMY OF ENVIRONMENTAL MODELS

Robert U. Ayres
International Research and Technology Corporation, 1501 Wilson Boulevard, Arlington, Virginia 22209

The Role of Models

Problems of the environment are essentially problems of production and consumption, as concerned with *real* physical materials and energy. These real physical materials must be derived from the natural environment where they are distributed unevenly. Their usage involves successive stages of processing and transformation which inevitably result in social costs (externalities), ranging from noise to the discharge of toxic waste materials. Similary, so-called "Final" consumption--that convenient abstraction from classical economics--is not final at all in terms of disposition of real materials and energy. On the contrary, consumption of material goods means in practical terms that the goods have lost their utility value and become wastes. But these still have to be disposed of and are still capable of causing very serious harm to the natural environment and to man, depending upon the location and method of discharge or disposal.

In short, a whole collection of new problems associated with stocks and flows of physical materials and energy has come to the fore. They were with us all along, but in the 1930's other problems associated with organizing the economy and fully utilizing its resources were far more urgent. Natural resources, on the other hand, are becoming painfully scarce in the industrialized world. Many of the most abundant natural resources of the earth have already been dissipated, not to say wasted. The surface of the earth still has abundance to offer, but we must dig deeper, scrape the bottom of the ocean, or look at more remote areas of mountains, deserts, and jungles. Extracting these resources is creating newer and more serious problems also. Delicate ecosystems such as the Arctic tundra or the tropical oceans are beginning to show adverse effects from this intensification of digging, drilling, and quarrying. Mine wastes, oil leakage, combustion products of a vast variety of types and kinds of pollution are fouling our environment, and making survival impossible for many harmless species of plants and animals which formerly shared the earth with us. Some have even questioned whether human life itself can survive for long amidst this environmental carnage.

No doubt, some of the immediate fears of resource exhaustion are overblown, but it is not our purpose here to evaluate their validity. It is enough to say simply that the "new" problems facing economists in the 1970's and 1980's are intimately associated with the real properties of physical materials and energy, and above all, with their stocks and flows--that is with their physical quantities. To deal with these problems we need first of all an appropriate economic theory. The conventional paradigm addresses the economy as a set of relationships between production, investment and consumption expressed in monetary terms, and defines its concerns as determining conditions for maximizing consumer utility and social welfare by optimizing these relationships. But another paradigm is needed in which the economy is viewed as a set of transformations of physical materials from the raw state through successive stages of extracting and processing to goods and services, and finally to waste flows. Even physical dispersion and biological impacts must be considered. The problem of optimization is correspondingly broadened. This broader theory must address the problem of production of externalities as well as economic services, and the allocation of such externalities. It must deal with the problem of defining and maximizing social welfare subject to resource supply pervasive constraints, laws of thermodynamics, and the existence of externalities resulting from waste residuals; and it must provide theoretical tools to facilitate our understanding of the appropriate mechanisms for managing the economy.

One characteristic of the "new" problems in environmental economics is that they are increasingly at the "micro", rather than the "macro" level of aggregation. Resource and environmental concerns tend to involve consideration of technological particulars, as contrasted with interrelationships among broad aggregates such as population or Gross National Product.

This increasing concern with detail is characteristic of the development of any science. In the early stages of development of theoretical chemistry, it was convenient to proceed by lumping all the chemical elements together, calling them "matter" and looking for generalized "laws of matter". But the number of valid inferences that can be made from this simple model is quite limited. Each element is different, each has different properties, each reacts differently from the others. Sooner or later the chemist is forced to recognize and take into account these differences by developing a more elaborate model.

However, the chemist continues to consider molecules essentially as complete entities. These are the objects of his research. It is precisely the combinations between atoms (of similar or dissimilar species), which are governed by electromagnetic forces, that chemistry is all about.

Note that the analytical methods of chemistry are of no value in studying reactions that occur within the nucleus of a single atom. These are governed by different--stronger but shorter range--forces which have essentially no influence on the interactions between atoms and molecules. Conversely, the electrical forces which govern inter-atomic relations have no measurable effect on the probabilities or rates of nuclear reactions. The two classes of phenomena are virtually independent of each other, though nevertheless governed by the same fundamental physical laws.

On the other extreme, consider the gravitational forces that control the motions of stars and planets. These are the only forces in the universe that are effective at truly long distances. But, by the same token, the gravitational forces are incredibly weak by comparison to electromagnetic forces. Only when enormous numbers of particles are collected together as "mass" is the gravitational effect significant--whereas the electrical forces are cancelled out at a distance by the fact that positive and negative charges are present in equal numbers. The laws of chemistry, then, have little to say about the motions of cosmological objects. Similarly, astrophysics contributes little to chemistry.

Each branch of science lumps together and aggregates "over" the objects and forces that are too weak or too short range to influence the phenomena with which it concerns itself. However, it also aggregates into categories those objects and forces with which it is concerned. Chemistry aggregates atoms and molecules by species. It does not examine single atoms. Similarly, other sciences such as physics, astronomy, and biology tend to classify their objects in such a way as to distinguish differences that matter from differences that do not matter at that level of aggregation.

Aggregation, ther, is at the heart of theoretical science. If an investigator examines only individual cases, in an individual way, patterns are indistinguishable and one is soon lost in a sea of particulars to which no general significance can be attached. On the other hand, if aggregation is carried too far, unlike elements are lumped together, essential differences are obscured and again, the expansion of knowledge is limited.

The environmental or social scientist's problem in this respect is obviously more complex than that of the chemist, who has to deal with a very limited number of clearly defined elements, with known atomic structure, which he combines or separates in endless ways. The environmental or social scientist, on the other hand, has no "unit" of absolutely fixed value or quantity. Measures of utility or value are ambiguous. Even physical measures of the quantity of a commodity (tons or cubic feet) fail to take account of physical transformations, not to mention variations in the quality. Not only is everything influenced by everything else, but everything fluctuates in relation to everything else.

In order to find answers to many of the pressing problems of an era of rapid technological change, an environmental economist must be able to carry out analysis at a level of aggregation that is appropriate to take into account the widely different *resources, materials, forms of energy and production processes* to which technological changes specifically apply.

A list of examples of "new" problems facing economists arising from the resource-environment-technology interface could be made arbitrarily long. Almost every major technological decision has a resource/environmental dimension. The controversy over the SST is an excellent illustration. To build and operate such an aircraft will result in increased demands for hydrocarbon fuels, and it will result in physical disturbances to the stratosphere that may ultimately affect the intensity of both ultraviolet and visible solar radiation on the Earth's surface. All of these impacts have potential economic consequences of significant magnitude, which require assessment.[1] Similarly, problems arising initially out of perceived resource-needs immediately reveal technological and environmental aspects. Thus, the exploitation of Alaska's north slope involved building an enormous north-south pipeline across Alaska, with immense potential for environmental disturbance. Proposals to exploit Colorado oil shale or Wyoming-Montana coal are seen to require diversion of large amounts of scarce water away from traditional agricultural uses. The proposals to solve a resource problem by relying more heavily on nuclear power, especially "breeder reactors" and plutonium reprocessing, are also evidently fraught with environmental risks.

The history of the last few years has been--and undoubtedly of the next decades will be--increasingly preoccupied by the need to choose among and between complex, expensive and uncertain technological programs; each of which involves large potential environmental risks and hazards as well as possible benefits. The cheap alternatives and easy choices are no longer available.

And the factors which must be weighted to arrive at rational choices are intrinsically concerned with detailed technological and environmental questions. What is the marginal impact on the human environment of one unit more (or less) of mercury? or PVC? What is the net environmental benefit of electric cars using nuclear power vis-a-vis ICE powered cars using gasoline? What if we burn coal to make electricity in large power plants in remote areas vis-a-vis converting it to gas and burning it in local "total energy" installations? How much will it cost to desulfurize coal? oil? What are the potential markets for by-product sulfur? Etc., etc.

Lawrence Klein has defined a *model* as a "schematic simplification that strips away the non-essential aspects to reveal the inner workings, shape, or design of a more complicated mechanism".[2] Aggregation is the key to model design, just as it is the key to theoretical science in a more general sense. The fact that a model cannot hope to reproduce "all" the details--even the more important ones--of a complex reality is an inherent limitation on what can be accomplished by it. Yet its comparative simplicity is also a strength. An excessively detailed model would be cumbersome to handle and expensive to maintain, yet still imperfect. On the other hand, the simplification of reality implicit in a model can be a trap, for if the model omits key factors that may have a determining effect on possible outcomes, it can depart too far from reality and lead to false conclusions. It is all too common for even experienced investigators (who should know better) to be hypnotized by the neat rows of figures emerging from a computer and mistake them for a portrayal of real facts.

Central to the design problem, too, is the decision of what factors the model should explicitly take into account. This judgment is determined by the questions the model is designed to answer. If the investigator wants to know how fast DDT is building up in the ocean, he may project DDT use in cotton farming and malaria control. This can be useful, although it does not tell him where the effects will be concentrated or which species will be affected. Its predictive accuracy, of course, hangs on the accuracy of the projections of the two aggregates: cotton production and public health use. If the tradeoff between malaria control and overpopulation is to be explored--by country--a much more detailed analysis of alternate strategies is needed. To accomplish the practical purposes of applied environmental analysis, clearly, we must build computerized accounting and optimization models to reflect a wide variety of such factors.

Qualitative vs. Quantitative Models

The first and most important distinction that needs to be made is between qualitative and quantitative models. The term "qualitative" may seem inappropriate as applied to models, but it is not. Diagrams and pictures--said to be "worth a thousand words"--are clearly models, by Klein's definition. (Even a photograph is a "model", since it represents a 3-dimentional dynamic reality in a 2-dimentional static form.) For that matter, a verbal description of a real event is also a kind of model. Qualitative models can be highly precise and rigorous in expressing certain types of information. A classic example is the famous periodic table of the elements, developed by Mendeleyev. It is clearly a model, and clearly qualitative. There are no measures involved.

Despite the obvious importance of qualitative models, the remainder of this paper will be concerned explicitly with quantitative models.

Simulation vs. Optimization Models

A second fundamental dichotomy can be drawn between simulation (or forecasting) models and optimization models. While both types are applicable in economics, the latter type is more fundamental to the discipline, whereas physical models are more likely to be of the former kind. Indeed, economics has generally been defined as the study of optimal allocation of scarce (limited in availability) resources among competing ends or uses (in ordinary language, this process is often simply called "economizing").

In particular, classifical economics is concerned with the allocation of investment capital among competing projects and localities, the allocation of income among competing expenditive categories (or means of achieving satisfaction), and so on. The newer problems of economics, as already noted, concern optimal allocation of natural resources among sectors of society, selection of technologies to maximize desired outputs and minimize costly inputs and/or costly wastes; selection of optimal pollution abatement strategies, investment schedules, etc.

Static vs. Dynamic Models

A third key distinction is between static and dynamic models. The static/dynamic distinction concerns the treatment of time. In a static model, time is not a variable: the solution is valid either for a particular point in time (only), or for *all* time, depending on whether the exogenous variables of the problem are themselves time dependent or not. "Cross-sectional" survey data is often used. In a dynamic model, time is an explicit variable and the solution evolves with time. Longitudinal (time-series) data is appropriate. Clearly the dynamic optimizing case is most general, but is also most difficult to formulate (and to compute). Static non-optimizing models are of comparatively little importance. The only significant example I know of in economics is the input-output model. I know of no good examples in the physical sciences. Combining the two dimensions, there are four major categories:

- static simulation
- dynamic simulation (forecasting) models
- static optimizing models
- dynamic optimizing models.

Causation vs. Correlation Models

Quantitative models may also be divided along another axis, depending on the use of phenomenological causality. This is not a distinction that can always be made cleanly by an outside observer, since it sometimes depends on the modeller's intentions. There is a wide spectrum. At one extreme one finds "blind" extrapolation of exponential curves as straight lines on log-paper--where no strict causality is even suggested and the forecaster assumed (in effect) that the curve has a kind of independent life. At the other extreme is the completely analytic model where everything is explained in terms of a fundamental physical theory, such as the "laws of gravitation". Obviously even fundamental theories are not unchangeable. (Too many have been upset during the present century for us to feel confident that we know all the basic laws governing matter and energy, still less living organisms.) Thus dependence on "causality" is always relative.

Econometric models, based on correlative relationships between variables determined by statistical analysis of time-series data, tend to be weak in causality. In a sense, the use of sophisticated statistical methods can be a substitute for understanding underlying mechanisms and relationships. (This is not necessarily the case: a good theoretical model can be improved by the application of refined statistical techniques for empirical estimation of key parameters. But often statistical means are employed to select relationships between variables precisely because fundamental theory is lacking; indeed, the theory may develop more rapidly as a consequence of such analysis.)

Realistic vs. Abstract Models

Causal models, based on fundamental theory--as opposed to correlative models developed by statistical analysis of empirical data--may be either realistic or abstract. In the latter case they are intended to represent real phenomena and to assist either in forecasts or in determining optimum arrangements. On the other hand, abstract (data-free) models are intended only to generate "theorems", elucidate limiting cases, and so forth. They tend to be deliberately oversimplified. Much of theoretical resource environmental economics in recent years has been concerned with exploring the properties of very simple models that (presumably) exemplify more general principles.

Short-term vs. Long-term Models

An important subsidiary distinction, applicable to realistic forecasts only, must be made between *short-term* and *long-term* dynamic simulation models. The distinction is extremely important in practice, yet often overlooked (or not understood) even by many practitioners. The difference hinges on how data is used in the model and how the results are interpreted. Briefly, long-term models are concerned with moving averages or trends, in which temporary departures from equilibrium are deliberately ignored. Indeed, the more precisely calibrated the model is for use in short-term forecasts, the faster it will depart from the long-term trends. Conversely the more closely it is tied to long-term trends the lower the correlation with short-term fluctuations. Hence fluctuations in the input (i.e. historical) data are regarded as "noise" and are normally smoothed over. On the other hand, short-term models are precisely concerned with the fluctuations away from equilibrium. Hence they tend to utilize *all* historical data, with the smallest possible time increments--usually quarterly--and, as a rule, recalibrate and recompute after each new set of data points are added to the series. And because the non-equilibrium aspect is vital, multiple correlation regression analysis is heavily used in developing the equations.

The important point here is that short-term models are *predictions* because they take off from an actual set of initial conditions, such that all values of variables and parameters are guaranteed to be realistic, at least, at time zero. The predictive value declines fairly rapidly as the forecast horizon is extended, of course, because the starting point is always off-equilibrium.

Long-term models, on the other hand, do not give predictions, but are used instead to make *projections* usually in sets of possible alternatives). A long-term model has no predictive value even in the short-run, because it is concerned with trends and smoothed averages. These are seldom in agreement with actual current values of the model variables. And because equilibrium conditions are mainly of concern, it is reasonable to depend heavily on accounting identities (e.g., input-output relationships, materials, energy balances, etc.) which can be relied upon to change fairly slowly, if at all. The purpose of a long-term model is to examine the quantitative consequences of changes in exogenous trends in parametric relationships or in constraints. Conclusions drawn from long-term models should always be explicitly *contingent* on the particular set of starting assumptions. (A contingent statement is always of the type: "if ... then ...". The assumptions are an intrinsic part of the statement.)

Because short-term and long-term models are used for different purposes (and supported by different institutional sponsors) the developers are often out of touch with each other and--at times--unjustifiably contemptuous of each other's methodologies. In particular, there is a tendency for each to encroach on the others' domain, rather than to develop a synergistic dialog. But it is becoming increasingly urgent that such a dialog be initiated, both to minimize duplication of effort and rediscovery of the wheel and for more fundamental reasons. The latter have to do with the need to develop realistic long-term dynamic optimizations in which short-run departures from equilibrium play an explicit role.

For the moment it is worth noting, simply, that realistic optimization models currently tend to draw more on engineering and physical information than on statistical (time-series) analysis--which may explain why econometricians have largely ignored this area in the past.

Levels of Aggregation

Considerations noted earlier suggest that one useful way of further subdividing realistic models is by level of aggregation. There exists a natural hierarchy of aggregation levels in economics, each level useful for some particular purpose. Most highly aggregated (call this Level 1) is the model based primarily on such broad measures as total population, total labor force, unemployment rate, gross national product, gross capital formation, private consumption expenditures, wholesale and consumers' price indexes, rate of price inflation and so on. Non-economic models at the same level would introduce total energy flow, biomass, etc. Some of these aggregates, notably population and labor force, can be estimated for a number of years ahead because birth and death rates change relatively slowly, and age distributions of the population can be projected with fair accuracy.

Beyond these pivotal aggregates, forecasts of economic quantities become increasingly difficult and have to be based on a priori assumptions, such as the proportionality of inputs to outputs or the assumption that relationships between the various quantities that have held true during past periods of time will continue to hold true in the future. Such relationships often take the form of equations, by which, if certain macro-variables such as population, labor force and productivity are assumed, the other quantities can be estimated. The trends projected by such techniques are more reliable for short-term forecasts than for long-term ones; and therefore, as forecasts extend further and further into the future, they are likely to become increasingly unrealistic.

A special problem with long-term forecasts at this level of aggregation is that the key elements affecting long-term changes in the economy are not necessarily the same as those affecting the short term. For the long-term, the key elements include technological changes, possible raw material shortages, rising energy costs, material substitutions, changes in social customs, changes in the educational level of the population, environmental deterioration, and many other factors not explicitly accounted for in the aggregates generally used in Level 1.

A second level of aggregation (call it Level 2) involves dividing up the economy by *industry sector* and/or *region*. A familiar example of this is the input-output model which takes the form of a matrix recording the pattern of flow of materials and energy (or the pattern of purchases and sales) between industry sectors, between each sector and the government, and between each sector and the final customer. Such a table does not identify the particular commodities or energy forms that flow into and out of the sectors, nor the transformations that take place in the production processes, but it accounts for all inflows and outflows *in total*. These inflows and outflows must balance, both for the system as a whole and for each individual sector after accounting for waste and for materials drawn from the environment.

The development of input-output models provided for the first time a comprehensive view of the *structure* of the economy, like a still photograph that catches an action in mid-motion. These models facilitated studies to be made that had formerly been extremely tedious, if not impossible. With them one could determine the effects a change in one sector might be expected to have on the other sectors. For example, if automobile size and weight are reduced, the direct effects on the iron and steel, coal mining, petroleum refining, glass, nonferrous metals, synthetic rubber, chemical, machine tools, and many other sectors can be traced. But beyond these direct effects are secondary and tertiary effects: the reduced demand for intermediate products entering into the automobile industry affects communications, transportation, electric power, and so on. The effects ripple through a maze of inter-relationships.

For some industries the level of aggregation used in published input-output tables--even if regionalized--is still much too broad for accurate analysis. For example, the sector "Industrial Chemicals" includes a wide variety of products made from different raw materials by different processes and used in different sectors. Thus benzene is derived both from coal and from petroleum. It is used in petroleum refining (to gasoline), in manufacturing synthetic rubber, in making the plastic styrene, and in many other chemicals. A shift in the proportions of these products within the sector can alter significantly the inputs and outputs for the sector.

At the commodity level of disaggregation, it is apparent that the same commodity can, in many cases, be produced by several alternative processes. An example is the production of PVC bottles. At least 20 different processes may be involved in PVC manufacture and these can be combined in more than 60 different ways--each with different environmental impacts. In other words, there are over 60 possible *chains of processes* leading from raw materials to finished PVC, all requiring different inputs and yielding different wastes. A study of the environmental consequences of regulations affecting process technology or energy would need to take these alternative chains of processes into account. To deal with problems where this level of detail is unavoidable requires a still higher level of disaggregation (Level 3).

Determinism vs. Uncertainty

A final distinction of utmost importance must be made between models that are endogenously deterministic with fixed inputs (in the clockwork sense) and models that explicitly provide for stochastic or irregularly variable inputs. Variable inputs may be distributed according to different rules, ranging from normal (Gaussian) or log-normal distributions to *ad hoc* heuristic "scenarios" *based on extra-model intelligence*.

In the case of physical models stochastic or normal distributions are common. For instance, the "mix" of local weather conditions, genetic variability, or other factors is likely to be subject to a normal type of distribution. Apart from this, however, indeterminacy is not a serious limitation for physical models since it comes into play only at the atomic or sub-atomic level of disaggregation. [Indeterminacy Principle, formulated by Heisenberg, states that the product of uncertainties of complementary variables such as momentum and position will always exceed a specified minimum value (called Planck's constant, h).]

In the case of economic, social or political models the situation is significantly less favorable for the modeller, however. Here the indeterminacy principle becomes a factor if one attempts to predict the behavior of individuals, committees or structured organizations (including governments) having a small number of effective decision-makers. This is a logical implication of the free-will of the individual. But, even if humans were actually instinctually pre-programmed, in the same sense as insects, an indeterminacy principle would still be applicable because it is clearly impossible to monitor an individual human's behavior (including thoughts) closely enough to predict his or her actions without disturbing the object of the surveillance to the point of affecting those actions significantly.

To deal with indeterminacy in the realm of human behavior it is convenient to introduce "policy" variables (or parameters) in the models. Rather than trying to predict what human behavior will be, which is impossible where a small number of effective decision-makers are involved, the model must be formulated to explore the implications of alternative decisions or "policy options".

Mapping Model Types to Issues

Space limitations do not permit a detailed exploration of this topic. A few brief comments must suffice to conclude this paper. How can one decide what type of model is most appropriate to a given policy issue? The foregoing taxonomy constitutes a kind of hierarchical checklist for the classification of *models*. In effect it defines a large number of possible "pigeon holes". On reflection, it is clear that the same screening process can also be applied to *problems* by examining the relevant variables and relationships:

- Are the pertinent data quantitative?
- Is the question one of prediction? Or is it a question of characterizing the best (optimal) solution?
- Is time an explicit variable?
- Is there an underlying phenomenological theory available? Or must one rely on observed correlations between independent observations?
- Is realism desired? Or is it the object of the exercise to deepen ones understanding of the fundamentals by systematic simplification?
- If time is a variable and realistic simulation is desired, is the time-scale short or long?
- What is the level of aggregation at which the key phenomena are observable (viz. National? sectoral? regional? commodity? process?).
- Are there stochastic or random elements in the problem? Is the behavioral response by individual decision-makers or small groups of decision-makers a factor in the problem?

Disregarding the last three items for quantitative models there are 12 possible combinations of the various characteristics noted above, of which 8 or 9 (at least) seem to be relevant (i.e. the boxes are occupied). For two of the categories a further short/long subdivision seems called for. Any of the cases may be at any level of aggregation and may involve stochastic or human choices.

	REALISTIC		NON-REALISTIC
	Non-causal (Statistical)	Causal-Empirical	Causal-Abstract
Static Simulation	?	X	X
Dynamic Simulation	Short Long	Short Long	X
Static Optimization		X	X
Dynamic Optimization			X

As noted above, classifications are not always unambiguous. For instance, an "equilibrium" air pollution dispersion (e.g. "plume") model would certainly be classed as a causal-empirical, but it is not quite clear whether the term "static" or "dynamic" is applicable. A pollution forecasting model utilizing empirically determined pollution coefficients for highly aggregated sectors would certainly be classed as static-simulation, but there might be a question as to whether truly causal relationships are used. If the pollution output for a sector were developed based on more detailed process-level analysis, explicitly incorporating materials and energy balances, there would be no ambiguity, of course.

As a matter of possible interest, SEAS belongs in the causal-empirical-dynamic simulation (long-term) category.[3] The Materials-Process-Product Model (IR&T)[4] and the Russell-Spofford Model (RFF)[5] probably belong in the causal-empirical static optimization. Examples of abstract models in the field of biology, ecology, and environmental economics are quite plentiful. However, realistic dynamic optimization models have not yet been developed to my knowledge.

1. A team of investigators composed of Wassily Leontief, Anne Carter, Peter Petri, and Joseph Stern, "Technical Report on the Study on the Impact of Prospective Environmental Issues and Policies on the International Development Strategy", prepared for the UN Center for Development Planning Projections and Policies Office, forthcoming.

2. Lawrence R. Klein, "What is a Model" (unpublished).

3. U.S. Environmental Protection Agency, Strategic Environmental Assessment System, Prototype Documentation, Phase III, 1975.

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A STOCHASTIC MODEL FOR SUBREGIONAL POPULATION PROJECTION

Peter M. Meier
Energy Policy Analysis Division
Dept. of Applied Science
Brookhaven National Laboratory
Upton, New York 11973

ABSTRACT

A stochastic method for the projection of subregional population is developed, to be used in conjunction with regional OBERS projections. The model is based on a Monte Carlo simulation and numerical integration technique to generate probability distributions of future population, given some analytical formulation of population density in urban areas, and is addressed particularly to consulting engineers who must make decisions on design capacity for waste treatment facilities.

INTRODUCTION

Projections of population, and the associated specification of service area, waste flows and pollutant loadings, lie at the very heart of the current national effort to reduce water pollution. Yet, as the recent controversy over excess capacity in interceptors has amply demonstrated,[1] the level of competency current in the environmental engineering profession in matters of socioeconomic planning is far from adequate. This deficiency is all the more serious in light of some of the very sophisticated optimization and design techniques employed in the engineering of the pollution abatement facilities themselves; it clearly makes little sense to devote substantial resources to detailed design and engineering optimization if the initial premise of design capacity and expected loadings is in substantial error. In view of the crude methods used to project population,[2] and the rigid use of design standards derived decades ago,[3] it should come as no surprise that a number of recent investigations have found fault with current facility planning practices. Indeed, it is a sorry reflection on the profession that the current EPA guidelines for planning treatment facilities find it necessary to provide sample calculations of a present worth analysis.

In this paper, we focus on one particular area of socioeconomic planning, population projection. The intent here is to illustrate some lines of analysis that might profitably be applied to any large public sector capital investment, but with particular emphasis on the planning of waste treatment facilities. Experts in mathematical modelling will find little in the way of sophisticated analytical formulation, but then its content is addressed to the practicing professional. Indeed, the most important criterion for the successful development of a modelling technique is the degree to which it is consonant with the ability of the consulting profession to apply it, and the ability of the public and the political process to understand its assumptions. Highly complex models will not aid the planning process if only their originators can fully use them or fully understand them.

THE OBERS PROJECTIONS

The OBERS projections of population and economic activity, prepared by the U.S. Department of Commerce and the U.S. Department of Agriculture for the Water Resources Council,[4] are now in fairly broad use as a basis for planning activities by Federal Agencies. And the U.S. Environmental Protection Agency (EPA) now requires that plans prepared under Section 201 of PL 92-500 relate the proposed facility capacity, and the forecast population to be served, to the applicable OBERS projection. Unfortunately, the smallest spatial unit for which an independent OBERS projection is available is the Standard Metropolitan Area (SMSA), yet the service area of even many large regional wastewater treatment facilities often cover far less than an entire SMSA. There thus seems some need to develop a rational method of sub-regional population projection within the framework of the regional OBERS forecast.

The classical solution to this problem is the so-called step-down projection technique, in which the total regional growth is assigned to sub-regional areas on the basis of some deterministic allocation scheme.[5] Unfortunately, such simple allocation formulae tend to be quite inadequate for the level of disaggregation necessary, say, for interceptor sizing, which requires minor civil divisions or census tracts as the basic spatial unit. Moreover, the most obvious deficiency in current methods of population projection is their deterministic nature, even despite the widely known and accepted circumstance that most population projections prove to be in error.[6] The urgent priority, then, is to formalize the notion of the probabilistic population projection in terms suitable for use in design algorithms.[7] That, of course, demands expression of a population projection as a probability distribution, rather than as the currently adopted expedient of specifying a "high" and a "low" projection, with a "most likely" case somewhere in between. Indeed, given a probabilistic expression of population and a corresponding probability distribution of expected flows, a number of algorithms developed in the Operations Research field can quickly identify the correct investment strategy, taking into account scale economies, interest rates, and planning horizons.[8] This approach, however, can only be used if probabilistic projections are available; and until that occurs, one can hardly fault those who adopt the traditional hedge against uncertainty that rests on overdesign.

The two major objectives of this paper, then, are to develop a probabilistic approach to step-down projections, and to suggest a step-down procedure that rests not on simple arithmetic allocation ratios but on the overall patterns of regional population distribution, obtaining the subregional population of interest by integration of the chosen functional representation over the appropriate spatial limits.

In the interest of clarity, we shall use a simple exponential model of urban population density as the basis for exposition; more complex analytical representations would pose only additional computational effort, without change to approach itself.

THE DETERMINISTIC CASE

In order to develop the sub-regional integration procedure, consider first the deterministic case of the classic exponential model of urban population density,[9] given by

$$d(r,t)=d(o,t)e^{-\alpha(t)r} \qquad (1)$$

where d(r,t) is the population density at time t at distance r from the city center, d(o,t) is the population density at the city center, and $\alpha(t)$ is the density gradient at time t. The total number of inhabitants within some radius R is then given by the integral

$$P(R,t) = \int^{R}\!\!\int^{\theta} d(o,t)\ e^{-\alpha(t)r} r\cdot dr\cdot d\theta \qquad (2)$$

$$= \frac{\theta d(o,t)}{\alpha(t)2}\left[1 - (1 + \alpha(t))e^{-\alpha(t)R}\right] \qquad (3)$$

where θ is the sectoral angle of the city, in radians.[10]

Given this model, we note that changes in population can only be accommodated by changes in the density gradient $\alpha(t)$ and/or the central density d(o,t). As noted by Winsborough[11] or Guest,[12] for example, most american cities have indeed experienced declines in $\alpha(t)$ and d(o,t) over the past decades to accommodate growth, a phenomenon familiar as urban sprawl.

Suppose, then, we are given the OBERS projection population for some SMSA, say P(R,t), t=1,...,n. Suppose also that estimates of $\alpha(t)$ and d(o,t) consistent with the P(r,t) are available (more of which below). As indicated on the Figure below, any subregion within the SMSA can be defined in terms of a sector angle θ_j, and two radii R_{1j}, R_{2j}.

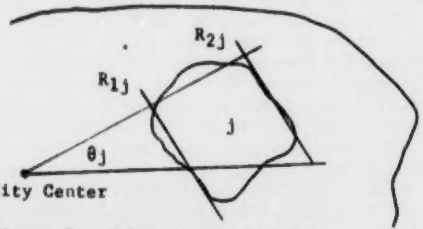

Figure 1: Subregion Definition

Then, if we define the subregional population at time t as $P_j(t)$, then the appropriate integral is clearly

$$P_j(t) = \int_{R_{2j}}^{R_{1j}}\!\!\int^{\theta_j} d(o,t)e^{-\alpha(t)r}\ r\cdot dr\cdot d\theta \qquad (4)$$

$$=\frac{\theta_j d(o,t)}{\alpha(t)}\left[R_{2j}e^{-\alpha(t)R_{2j}} - R_{1j}e^{-\alpha(t)R_{1j}}\right] \qquad (5)$$

If $\alpha(t)$ and d(o,t) were known with certainty, i.e. were deterministic in nature, then obviously $P_j(t)$, too, would be deterministic in nature, and specified completely by Equation (5).

DETERMINATION OF MODEL PARAMETERS

The first step in applying Eq. (5) for projection purposes is clearly to determine the model parameters of the base year, the starting point for specification of $\alpha(t)$ and d(o,t) through time. Indeed, even if we were subsequently to adhere to the deterministic form, one encounters the problem of estimation error in model specification; because any model that is reasonably tractable will not fit the observed data exactly. Suppose, for example, that for some urban area a series of population density - distance values were available, say one data point for each of k SMSA census tracts. Because these data points will not exactly fit the hypothesized exponential model, a more reasonable model specification, to replace Eq. (1), would be

$$d(r,t) = d(o,t)\ e^{-\alpha(t)r}\cdot u(r,t) \qquad (6)$$

where u(r,t) is some random variable of zero mean. Then, under the assumption that log u(r,t) is normally distributed with constant variance σ_t, the logarithmic transformation

$$\log d(r,t) = \log d(o,t) - \alpha(t)\cdot r + \log u(r,t) \qquad (7)$$

can be used to give unbiased estimates of $\alpha(t)$ and d(o,t) for any historical time point. Such a regression can obviously be used to estimate σ_t, and typical values of R^2 for this method of model estimation lie in the range of 0.6 to 0.8.

Unfortunately, the constant variance condition is rarely satisfied in practice, and the sampling variability proves to be quite high.[13] Yet, the preparation of a complete set of data points, say one per census tract, for even an average sized SMSA involves an inordinate amount of work, since the census tract areas are not generally available. To be sure, there are proprietary sources of census tract areas, but these are expensive and would, in all probability, not be used by a consulting firm.[14] And, other methods of area determination, and center of gravity and distance estimation, all introduce additional measurement error, with the result that simple regression estimation may be rather poor.

There are, fortunately, some other methods of parameter estimation, and one recent application of the exponential density model derives a numerical estimation procedure requiring knowledge of only the SMSA and Central city populations, areas, and average radii.[15] For a circular city, it can be shown that $\alpha(t)$ is given by the root of

$$y(\alpha(t)) = \frac{P(R_c,t)}{R(R_A,t)}\cdot\frac{1 - (1 + \alpha(t)\cdot R_A)e^{-\alpha(t)R_A}}{1 - (1 + \alpha(t)R_c)e^{-\alpha(t)R_c}} - 1 = 0 \qquad (8)$$

a root that is readily computed by the Newton-Raphson technique and where R_c is the average radius, $P(R_c,t)$ the population of the central city, and R_A the average radius of the SMSA. More complex spatial geometries can also be handled by a similar expression, although a numerical determination of an elliptical integral may be required. But most consulting engineering firms now have access to advanced computing facilities, either via remote batch station or interactive teletype, and these facilities offer documented program and subroutine packages for almost every conceivable numerical method or numerical integration.[16]

The final step in the deterministic model is to project the model parameters $\alpha(t)$, d(o,t) into the future. However, since P(R,t) is given by the OBERS projection, only one of these two parameters needs to be determined; for example, suppose one were to specify d(o,t), t=1,...,n; then for each t, the corresponding $\alpha(t)$ is given by Eq. (3). Although we cannot solve Eq. (3) explicitly for $\alpha(t)$, one can again turn to a numerical solution procedure, and $\alpha(t)$ is in fact given by the root of

$$y(\alpha(t))=P(R,t) - \frac{\theta d(o,t)}{\alpha(t)^2}\left[1 - (1 + \alpha(t))e^{-\alpha(t)R}\right]= 0 \tag{9}$$

In general, for a model of spatial population distribution of g parameters, g-1 parameters must be projected into the future, the g-th being determined by the specified parameters and the OBERS projection $P(R,t)$.

At this point, then, having a projection for $\alpha(t)$; $d(o,t),t=1,..n$, we can apply Eq. (5) to project the population of any subarea j. The beauty of the approach, of course, lies in the fact that one can generate projections for an entire set of subregions (by merely changing the limits of integration in Eq. (5)), projections which are not only all consistent with the overall SMSA projection, but also with each other. This is in contrast to the procedure followed in most regional plans for wastewater or water supply, where the population of each community tends to be projected separately, with total regional population given as the total (which may or may not agree with an independent projection for the region as a whole).

THE STOCHASTIC CASE

In addition to the measurement and model specification error discussed above, the most obvious source of uncertainty lies in the OBERS projection itself. These projections are based on certain expectations regarding national birth and death rates, inter-regional migration patterns, and shift-share analysis of regional economic activity; and, although the OBERS projections are generally regarded as methodologically sound, even their most avid proponents do not claim perfect foresight. To be realistic, then, even the OBERS projections must be expected to show error, once we have the benefit of hindsight. However, for purposes of this paper (and indeed for facilities planning under current EPA Guidelines), we can assume that the OBERS projections are the best in existence, and we shall simply assume that any uncertainty is sufficiently small in comparison to other sources that they may be ignored. Indeed, it should be intuitively obvious that the uncertainty associated with the projection of large spatial units is much less than projections of small regions, a notion fully supported by statistical evaluations of projection accuracy.

Given the premise, then, that the major source of uncertainty lies in our ability to accurately predict the distribution of population within the SMSA, what does this imply for our model? In terms of the exponential representation used in this paper, it simply means that the projection of $d(o,t)$ into the future (or, alternatively, of $\alpha(t)$), is a stochastic rather than a deterministic procedure. Thus, rather than specifying a single set of values $d(o,t),t=1,..n$ (which in turn specifies a single series of $\alpha(t)$, and subsequently a single deterministic projection for $P_j(t)$), we admit that for each time point, the value of $d(o,t)$ is in fact given by some probability distribution. This, in turn, implies that $\alpha(t)$ is also a random variable, as is $P_j(t)$. Thus, by generating a probabilistic statement for $d(o,t)$, one can also generate the desired probabilistic projection for $P_j(t)$.

Unfortunately, even using a model as simple as the one used here, analytical solution is quite intractable. That is, given a known probability distribution for $d(o,t)$, it is not possible to easily derive an expression for the probability distribution of $P_j(t)$. Indeed, even the relationship between the mean and variance of $d(o,t)$ and P_j is not easy to determine analytically, in view of the difficulty of explicit solution of Eq. (3). But even in the event that a model were chosen that allowed explicit solution of parameters, the effort of analytical solution would be beyond the capabilities of most non-mathematicians.

This type of situation, however, is almost ideal for applying the so-called Monte Carlo, or stochastic simulation technique. This technique simply repeats the projection procedure defined for the deterministic case some number of times, say q times; but each time the projection is repeated, a value for $d(o,t)$ is drawn from an urn which contains a set of $d(o,t)$ values that corresponds to the probability distribution chosen. The result is that the procedure generates q projections for $P_j(t)$; but since each projection depends on a different value of $d(o,t)$, $P_j(t)$ will also differ from projection to projection. In turn, the q projections for $P_j(t)$ define a probability distribution, whose moments can readily be calculated. Of course, the urn in a computer program is simply a subroutine that generates successive random values in accordance with the desired probability distribution.

A sample calculation will illustrate the procedure. Figures 2, 3, and 4 show the result of such a Monte Carlo simulation projection for part of the Trenton, N.J. SMSA. Figure 2 shows the distribution of $d(o,1985)$ and $d(o,2000)$, as generated by the random value subroutine; Figure 3 shows the distribution of $\alpha(1985)$, $\alpha(2000)$, and finally Figure 4 shows the distribution of sample projection values for $P_j(1985)$ and $P_j(2000)$. From this distribution of sample values, we compute the desired lower moments of the projection; the expected values in this case compute to

$$E[P_j(1985)]= 19600$$

$$E[P_j(2000)]= 21200$$

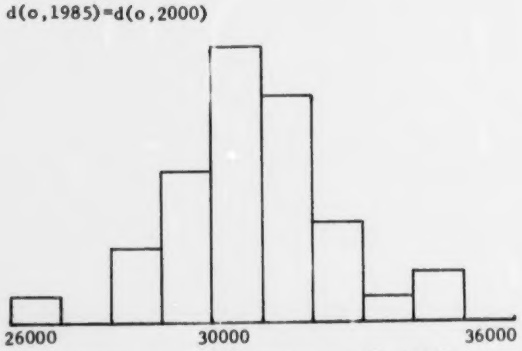

Figure 2: Distribution of d(o,1985)

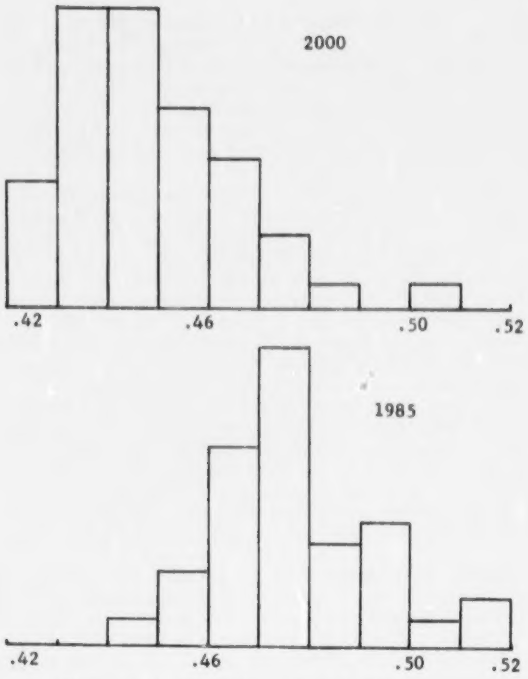

Figure 3: Distribution of $\alpha(t)$

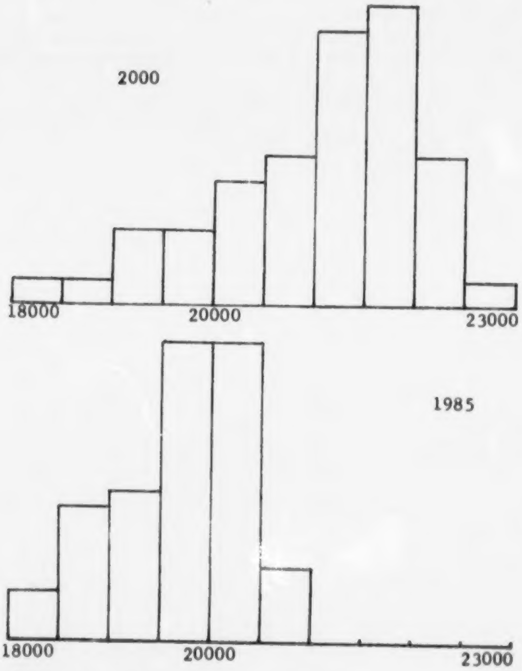

Figure 4: Distribution of $P_j(t)$

This particular series was generated by assuming a normal distribution for d(o,t); we note that the distribution of $\alpha(t)$, however, is skewed, as is the resulting distribution of $P_j(t)$.
Depending on the assumptions made for the distribution of d(o,t), different types of probability distribution would be generated for $P_j(t)$.

It could be argued that the procedure here is somewhat arbitrary, given the infinite number of possible probability specifications for d(o,t). However, a closer examination indicates that the definition of d(o,t) is little different from the definition of most of the parameters selected, say, in designing a treatment facility; the engineer applies his judgement and experience in selecting the major design variables, and, as he runs through the entire process chain, returns to make adjustments to previously selected design parameters so that the final design product has overall consistency. In a similar manner, then, an experienced planner makes judgements on the expected development of central population density, a judgement that would be based on analysis of land use developments in the region, likely trends in zoning, urban renewal, and central city revitalization efforts and so on. Different developments can readily be associated with different assessments of likelihood, from which a probability distribution of outcomes can readily be generated. The use of the model, then, forces the decision-maker to think about the factors that determine the distribution of population, a process that is not engendered by the more crude methods of fitting regression lines to historical data, or simply drawing arbitrary extrapolations.

CONCLUSIONS

In this brief exposition we have suggested some approaches to sub-regional population projections that should lie within the bounds of comprehension of the average consulting firm. The emphasis has been on developing the theme of the stochastic population projection, and the imposition of a planning framework that forces the individual who makes decisions on design capacity of treatment facilities to give more detailed thought to the underlying forces of urban and regional population growth patterns than is now customary. More complex representations of urban spatial growth than the one employed here could readily be incorporated, and indeed the computer package is designed in such a way as to encourage the planner to experiment with alternative formulations. Hopefully by such experimentation and simulation, the decision-maker gains a better understanding of the relationships between planning assumptions and the sensitivity of population projections used as a basis for large capital investments, in addition to providing the design engineer with a rigorous definition of uncertainty in terms of well-defined probability distributions.

ACKNOWLEDGEMENT

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The content of the paper, however, reflects the personal judgements of the writer, and should not necessarily be viewed as the position of either the Brookhaven National Laboratory, or the U.S. Energy and Research Administration.

NOTES

1. See e.g., Urban Systems Research and Engineering, "Interceptor Sewers and Suburgan Sprawl: the Impact of Construction Grants on Residential Land Use", Report to CEQ, Sept., 1974; and e.g. editorial comment in recent issues of the WPCF Journal, especially Vol. 47, No. 7, p. 1823 (July 1975).

2. One need only scan the most recent texts in the field, e.g. Metcalf and Eddy's recent book, or recent

editions of Fair, Geyer, and Okun, to ascertain the primitive nature of current techniques of population projection in comparison to the remaining facets of engineering design.

3. For example, R. Zanoni and R. Rutkowski, in,"Per Capita Loadings of Domestic Wastewater", *J. WPCF*, Vol. 44, No. 9, p.1757 (Sept.1972), point out that the per capita loading factors of BOD and Suspended Solids, still prescribed by many state standards for facility design, are based on wastewater characteristics of two and three decades ago, and often quite different to currently encountered values.

4. U.S. Water Resources Council, Washington, D.C., "OBERS Projections of Regional Economic Activity in the U.S., Series E Population, Vol.5, Standard Metropolitan Statistic Areas", April, 1974.

5. For an overview of these methods, see e.g. W. Isard et al., "Methods of Regional Analysis: An Introduction to Regional Science", MIT Press, Cambridge, Mass., 1960, Chapter 2.

6. P. M. Berthuouex, in "Some Historical Statistics Related to Future Standards", *Journal, Env. Engr. Div. ASCE*, Vol. 100, No. EE2, p.423, April, 1974, includes a very interesting analysis of the error distribution of population projections made by consulting engineers over the past few decades.

7. See e.g. Berthuouex and L. B. Polkowski, "Optimum Waste Treatment Plant Design under Uncertainty", *J. WPCF*, Vol. 43, No.9,p.1589 (Sept.,1970) for an illustration of engineering optimization given an input of specified probabilistic characteristics.

8. For further details on probabilistic population projections and their use in Environmental Engineering Design, see P. M. Meier, "Population Projection at Design Level", *Journal, San. Engr. Div., ASCE*, Vol.98, No. SA6, p.883 (Dec., 1972). The relationship between interest rate, scale economies, and projection uncertainty is given in P. Berthuouex and L. Polkowski, "Design Capacities to Accommodate Forecast Uncertainties", *Journal, Sanitary Engr. Div., ASCE*, Vol. 96, No. SA5, p.1183-1210.

9. This, of course, is the classic model of R. Clark, "Urban Population Densities", *Journal of the Royal Statistical Society*, Series A, Vol. 114, No. 4, p.490, (1951). Countless further empirical studies have confirmed the general validity of this model for all but oriental cities.

10. For definition and discussion of the spatial geometry of SMSA's, see P. M. Meier and M. McCoy, "An Analytical Approach to the Determination of Urban Population Density Gradients and its Application to Energy Planning Problems", Energy Policy Analysis Group, Brookhaven National Lab., Report BNL 20916, Jan, 1976.

11. H. Winsborough, "City Growth and Urban Structure", *Journal of Regional Science*, Vol. 4, No. 2, p. (1962).

12. A.Guest, "Urban Growth and Population Densities", *Demography*, Vol. 10, p. 53 (1973).

13. See Meier and McCoy, Note 10, *supra*, Chapter VIII.

14. The National Planning Data Corporation of Rochester, N.Y. has made census tract area determinations for all SMSA's using advanced electronic planimetry; however, use of this proprietary computer data base runs to several hundred dollars for an average SMSA.

15. Meier and McCoy, Note 10, *supra*, at p. 14.

16. Many firms, for example, have access to the national computing networks of the Boeing and McDonnell Douglas Companies via remote batch station, especially firms active in structural engineering.

17. The use of Monte Carlo Simulation in population projection is developed in Meier, Note 8, *supra*.

USE OF THE CLIMATOLOGICAL DISPERSION MODEL FOR AIR QUALITY MAINTENANCE PLANNING IN THE STATE OF RHODE ISLAND

Peter H. Guldberg
Walden Research Division of Abcor, Inc.
Cambridge, Mass.

Thomas E. Wright
Rhode Island Division of Air Pollution Control
Providence, R.I.

Audrey R. McAllister
Environemental Protection Agency
Boston, Mass.

Summary

An air quality modeling analysis was performed in preparation of an Air Quality Maintenance Plan (AQMP) for the State of Rhode Island.[1] The Climatological Dispersion Model (CDM), developed by EPA[2], was used to project future air quality levels and to test maintenance strategies for the years 1978, 1980, and 1985.

The choice of the CDM for maintenance analysis over the Air Quality Display Model[3] (AQDM) is discussed. The accuracy of the CDM is demonstrated, and suggestions for improvement of the model are made.

Introduction

In June, 1973, EPA published regulations[4] requiring all states to identify areas that might, as a consequence of current air quality and/or of the projected growth rate of the area for the next 10 years, have the potential for exceeding any National Ambient Air Quality Standard (NAAQS). States were also required to submit a detailed analysis of the impact on air quality of projected growth in each such designated Air Quality Maintenance Area (AQMA). Where NAAQS maintenance problems are identified by analysis, the states must submit a long-term Air Quality Maintenance Plan (AQMP) containing measures to ensure maintenance of NAAQS for a 10-year period from the date of submission of the plan. The submittal of long-term plans will be made according to time schedules to be published by the Administrator no later than July 1976. In the interim, EPA Region I is requiring states in their jurisdiction to submit attainment and short-term maintenance (i.e., 1975 to 1978) plans for Set I pollutants (SO_2 and TSP) only.

Based upon information supplied to EPA in 1974 by the Rhode Island Department of Health, Division of Air Pollution Control (DAPC), one AQMA in Rhode Island was identified by the Administrator as having the potential for violating NAAQS in the 10-year period between 1975 and 1985[5]. The boundaries of this AQMA are shown by the shaded area in Figure 1; they include 21 municipalities centered around Metropolitan Providence. The pollutants for which the Metropolitan Providence AQMA has been identified are Sulfur Dioxide (SO_2), Total Suspended Particulates (TSP), and Photochemical Oxidants.

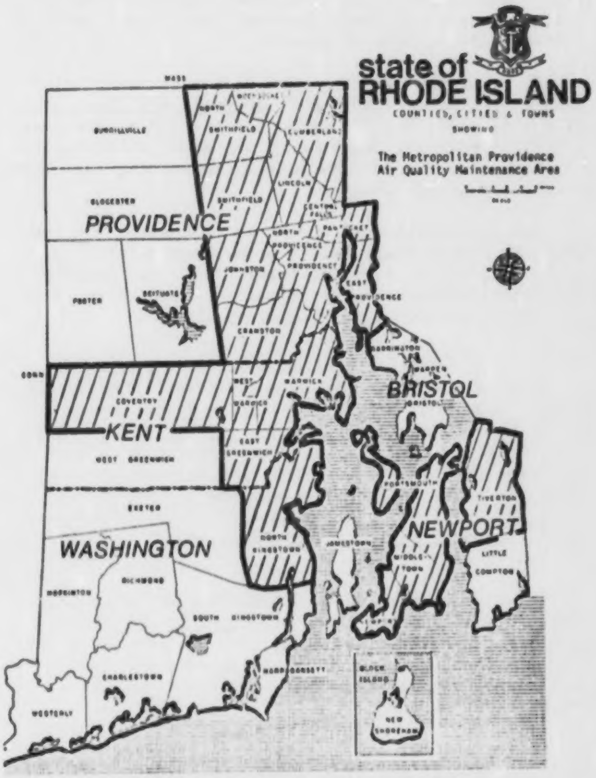
state of RHODE ISLAND
COUNTIES, CITIES & TOWNS
SHOWING
The Metropolitan Providence Air Quality Maintenance Area
MASS
CONN
PROVIDENCE
KENT
WASHINGTON
BRISTOL
NEWPORT
BURRILLVILLE
GLOCESTER
FOSTER
SCITUATE
NORTH SMITHFIELD
SMITHFIELD
CUMBERLAND
LINCOLN
CENTRAL FALLS
PAWTUCKET
NORTH PROVIDENCE
PROVIDENCE
JOHNSTON
EAST PROVIDENCE
CRANSTON
BARRINGTON
WARREN
BRISTOL
WEST WARWICK
WARWICK
COVENTRY
EAST GREENWICH
WEST GREENWICH
EXETER
NORTH KINGSTOWN
JAMESTOWN
PORTSMOUTH
MIDDLETOWN
TIVERTON
LITTLE COMPTON
RICHMOND
HOPKINTON
SOUTH KINGSTOWN
NARRAGANSETT
CHARLESTOWN
WESTERLY
BLOCK ISLAND
NEW SHOREHAM

Figure 1. AQMA with Potential for Violating NAAQS Between 1975 and 1985

Objectives of Study

Technical assistance was provided to the State of Rhode Island DAPC to develop an AQMP for the Metropolitan Providence AQMA. As a result of this work, the state submitted a draft summary of their short-term plan to EPA in January 1976. Air quality projections and control strategy analyses were performed for the years of 1978, 1980, and 1985 to:

> Determine areas in the Metropolitan Providence AQMA where annual NAAQS for SO_2 and TSP will be exceeded

- Evaluate control strategies which will ensure maintenance of standards in these areas through 1985.

An investigation of photochemical oxidants was not undertaken as part of this study.

Technical Approach

Air quality modeling analyses were performed to project future air quality levels and to test maintenance strategies. The work effort entailed the execution of the following tasks:

- The Rhode Island point source emissions inventory was updated to the base year of 1974, and the information was submitted to the NEDS data bank at EPA.
- Modifications to the CDM were made to allow for representation of stable atmospheric dispersion conditions.
- Utilizing the base-year point and area source emission inventories as inputs to the CDM, a validation of the model was performed by comparing predicted annual SO_2 and TSP levels for 1974 with measured air quality data in the AQMA from EPA's Storage and Retrieval of Aeormetric Data (SAROAD) system.
- The CDM was calibrated using the statistical relationship between measured and predicted pollutant concentrations derived in the model validation.
- Using data from the State of Rhode Island Land Use Plan[6] and methodologies outlined in EPA's AQMP Guidelines, growth factors were developed for projecting point and area source SO_2 and TSP emissions for 1978, 1980, and 1985.
- The above growth factors were applied to the base-year (1974) emissions inventories for 1978, 1980, and 1985. These projected base case emissions incorporate the effects of Federal New Source Performance Standards (NSPS) and the Providence Transportation Control Plan and assume full compliance with current state air pollution control regulations.
- Utilizing the projected inventories as inputs to the CDM, future annual SO_2 and TSP levels in the Metropolitan Providence AQMA were projected for the years 1978, 1980, and 1985. Based on these modeling projections, areas in the AQMA where annual NAAQS for SO_2 and TSP will be exceeded were identified.
- Control strategies were entered into the future air quality predictions through adjustments to the projected point and area source emission inventories. The CDM was used to evaluate the effectiveness of the various control strategies in maintaining annual NAAQS for SO_2 and TSP through 1985.

Description of Atmospheric Diffusion Model

Model Choice

Successful application of generalized models to specific emission sources requires definition of the source characteristics. The air quality maintenance analysis undertaken in the current study required an atmospheric transport and diffusion model capable of predicting annual average SO_2 and TSP concentrations at specified receptor points due to an array of both point and area emissions sources. In addition, the reactive nature of SO_2 necessitated the use of a model which could simulate pollutant decay processes as a function of atmospheric residence time. The two most widely used and accepted atmospheric diffusion models which met the above criteria are the Air Quality Display Model[3] (AQDM) and the CDM[2]. Both models are based on the Gaussian plume configuration, i.e., they simulate atmospheric transport and diffusion processes by assuming the concentrations of pollutants downwind within a plume generated by point and area source emissions can be represented by a Gaussian distribution in both the crosswind and vertical directions. Emissions sources are assumed to be continuous for the time analyzed. As the plume expands due to diffusion and turbulence, it is diluted and transported downwind, principally by the mean wind. The rate of expansion is characterized by a series of empirical dispersion curves which are dependent on the stability of the atmosphere, as determined in studies made by Pasquill[8] and reported by Turner[9]. A stability-dependent mixing height is also used to simulate diffusion processes in the atmospheric mixing layer.

The CDM differs in some respects from AQDM, which has been used extensively for simulation purposes. Although both predict long-term pollutant concentrations, the CDM determines emission contributions from area sources more accurately than AQDM, using numerical integration techniques. Effective emission heights for point sources are calculated in both models using the well accepted Briggs* plume rise formulae[10,11], and both models make use of an exponential decay term to simulate the reactivity of SO_2 with other atmospheric constituents. However, the CDM allows a realistic atmospheric stability-dependent power law increase in wind speed with height that is lacking in EPA's AQDM.

Finally, a validation study conducted at the National Environmental Research Center[12] has shown that the CDM yielded smaller errors than the AQDM, with concentration maxima and means nearer those of the measured data. For these reasons, the CDM was judged to be the model best suited to air quality maintenance analysis and therefore, was chosen for use in this study.

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*The original version of EPA's AQDM described in the user's manual[7] has been subsequently modified to replace the Holland plume rise equations with those developed by Briggs.

Model Modifications

The CDM model computes concentrations at receptor points which are assumed to be located in urban areas. The lower layer of the urban atmosphere is generally more unstable than the corresponding adjacent rural atmosphere. In fact, the turbulence and heating present in the lower urban atmosphere precludes the occurrence of stable atmospheric conditions associated with nighttime radiational cooling in the rural environment. To account for this effect, the CDM uses empirical dispersion coefficients associated with less stable atmospheric conditions in computing pollutant concentrations. While this procedure is correct when both receptor and source are located within the urban environment, it was felt that some adjustment was necessary in order to model the rural portion of the Metropolitan Providence AQMA. Rural receptors are by definition located far from the urban core, and the travel time from the source to the receptor is dominated by the rural component. Thus, in calculating pollutant concentrations at rural receptor sites, the dispersion of emissions was determined using the empirical dispersion coefficients of Pasquill[8] directly without adjustments for the urban environment. This allowed modeling of stable atmospheric conditions when applicable in the rural environment. In addition, the Briggs plume rise formulae used in the CDM were updated to include equations for plume rise under stable atmospheric conditions.

Model Input

The CDM accepts as input the joint frequency distribution of meteorological conditions, the average afternoon and nocturnal mixing heights, the locations and emission rates of both area and point sources, and the locations of the desired receptor points. At each receptor, the concentration due to each point and area source is calculated. These calculations assume transport and diffusion processes which represent the frequency distribution of meteorological conditions input to the model.

The basic meteorological input to the model consisted of standard "Day/Night STAR" data from the National Climatic Center in Asheville, North Carolina. Weather observations for Providence, Rhode Island (Station #14765) are taken hourly by the National Weather Service at Green Airport. These data, aggregated to eight observations per day and distributed as STAR data, are representative of the meteorological conditions for the State of Rhode Island. The result is a joint frequency distribution which gives the joint frequency of occurrence of a wind direction sector, wind speed class, and stability class. There are 16 different wind direction sectors, 6 wind speed classes, and 6 atmospheric stability classes. The CDM is well suited for AQMP evaluation since the NCC can provide "Day/Night STAR" data for any year at any station in the U.S. where daily weather observations are taken. Measured data in the joint frequency distribution are divided into two classes indicating their occurrence during either the day or night. This information is used along with factors input to the CDM, which estimate the diurnal variation of emissions, to more accurately predict ambient pollutant concentrations. The effects of seasonal variations in emissions on ambient concentrations can also be accounted for through the use of quarterly emissions data in CDM with quarterly "Day/Night STAR" data available from NCC.

For the model validation, in which predictions of annual concentrations of SO_2 and TSP in 1974 were made, the 1974 annual STAR data were used as input to the CDM model. To model future years, a 10-year climatological average STAR data set for 1964 to 1973 was used. Although use of STAR data from a particular year may have yielded higher predicted concentrations at some points in the AQMA, it was not possible to objectively determine the annual worst case meteorological conditions for the entire AQMA due to complex source-receptor relationships in the urban area studied. Therefore, climatological average meteorological data were judged to be the best representation of possible future conditions.

Model Validation and Calibration

For the purpose of verifying the accuracy of CDM in predicting annual average SO_2 and TSP concentrations for the State of Rhode Island, a model validation exercise was performed. This validation consisted of comparing air quality model predictions for 1974 with actual 1974 annual concentrations measured at 22 intermittent and continuous-monitoring stations throughout the AQMA. The measured data were obtained from EPA's SAROAD data file at the National Aerometric Data Bank.

Scatter diagrams of measured versus predicted 1974 annual average concentrations of SO_2 and TSP are shown, respectively, in Figures 2 and 3.

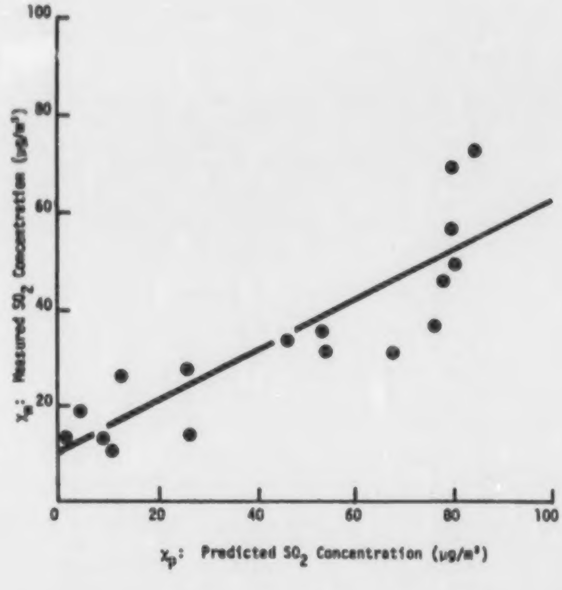

Figure 2. Comparison of Measured and Predicted 1974 Annual SO_2 Concentrations in the Metropolitan Providence AQMA

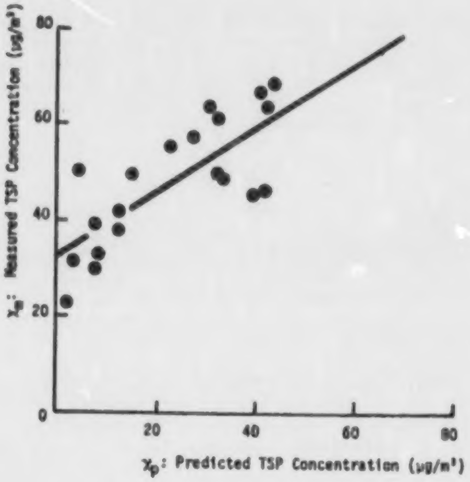

Figure 3. Comparison of Measured and Predicted 1974 Annual TSP Concentrations in the Metropolitan Providence AQMA

The correlation coefficients (r) between measured and predicted concentrations are 0.86 and 0.78, respectively, for SO$_2$ and TSP. These results indicate good correlation between these quantities and demonstrate the accuracy of the CDM in predicting air quality levels throughout the AQMA. The correlations may also be interpreted quantitatively, since r^2 is equal to the percentage of the variance of the measured concentrations that can be accounted for by a linear relationship with the predicted concentrations. These values are 74% and 61%, respectively, for SO$_2$ and TSP. The standard errors of estimate for the linear regression relationships were found to be 10.0 µg/m^3 and 8.3 µg/m^3, respectively, for SO$_2$ and TSP.

The purpose of a calibration is to adjust model estimates based on the relationship between measured (X_m) and predicted (X_p) concentrations determined from the model validation. This is accomplished by a linear regression on the validation data of which slope and intercept are then used as correction factors in making future predictions. Referring to the scatter diagram for SO$_2$ in Figure 2, the linear regression line of best fit was found to be $X_m = 0.52X_p + 9.9$ by the method of least squares. Referring to Figure 3 for TSP, the linear regression line was found to be $X_m = 0.67X_p + 31.9$.

These equations were used to calibrate the model for all future modeling predictions. Note that both lines have a positive intercept. There are three possible physical interpretations of these intercepts: (1) background pollutant concentrations, (2) systematic bias in the measured data, and (3) systematic bias in the model predictions. For particulate matter, 31.9 µg/m^3 is within the normal background level range due to road dust, pollen, and other fugitive dust sources, supported by the lowest measured annual average TSP value in the State in 1974 of 23 µg/m^3 in Washington County. For SO$_2$, the background level of 9.9 µg/m^3 is supported by the lowest measured annual average value in the State in 1974 of 11 µg/m^3, in the town of Westerly.

Future Base Case Air Quality

Calibrated modeling predictions of future air quality levels indicate that the annual primary standard for SO$_2$ of 80 µg/m^3 will not be exceeded in the Metropolitan Providence AQMA through 1985. The maximum predicted concentration was 54 µg/m^3, occurring in the city of Providence in 1985. Even if the standard error of estimate of the SO$_2$ model predictions of 10.0 µg/m^3 is added to this value, the result is still well within the standard*.

Future TSP levels are also predicted not to exceed the annual primary standard of 75 g/m^3. However, TSP levels are predicted to exceed the annual secondary standard of 60 µg/m^3 by 1.4 µg/m^3 in the city of Providence in 1985. It should be noted that this increment is less than the standard error of estimate of the model calibration of 8.3 µg/m^3. Concentration isopleths and the predicted area of violation for this case are shown in Figure 4 as an example of results obtainable from the CDM.

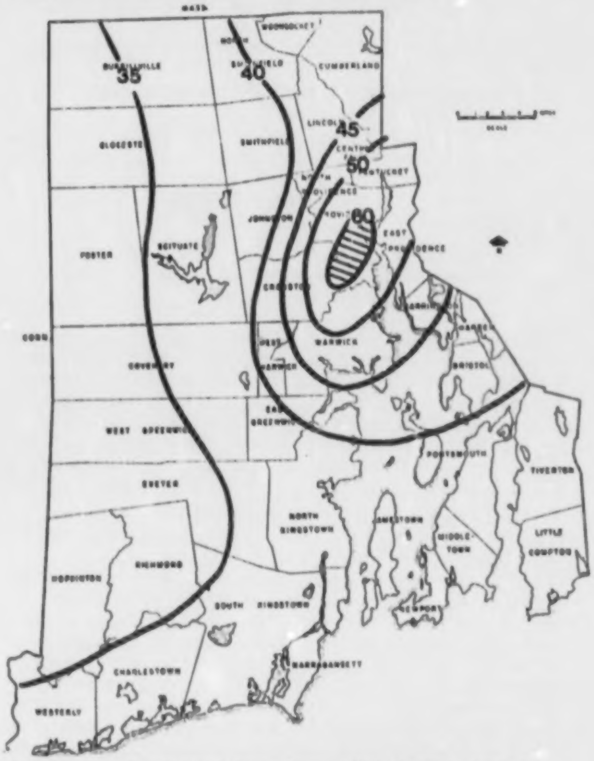
MASS
WOONSOCKET
NORTH
SMITHFIELD
CUMBERLAND
BURRILLVILLE
35
40
LINCOLN
45
GLOCESTER
SMITHFIELD
50
PAWTUCKET
NORTH PROVIDENCE
JOHNSTON
60
EAST PROVIDENCE
FOSTER
SCITUATE
CRANSTON
WARREN
CONN
WEST
WARWICK
COVENTRY
BRISTOL
EAST GREENWICH
WEST GREENWICH
PORTSMOUTH
TIVERTON
EXETER
NORTH KINGSTOWN
JAMESTOWN
MIDDLETOWN
LITTLE COMPTON
RICHMOND
HOPKINTON
SOUTH KINGSTOWN
NEWPORT
NARRAGANSETT
CHARLESTOWN
WESTERLY

Figure 4. Predicted Base Case 1985 Annual Average TSP Concentrations in Rhode Island (g/m^3)

The annual secondary TSP standard of 60 g/m^3 is to be used only as a guide in assessing implementation plans to achieve the 24-hour secondary TSP standard of 150 g/m^3. Therefore, an analysis was undertaken to extrapolate statistically the future base case annual average TSP concentrations predicted by CDM to 24-hour maximum values, using the techniques of Larsen[13]. The purpose of this analysis was to verify that the predicted TSP levels exceeding the annual secondary TSP standard in the AQMA imply violations of the 24-hour secondary standard and hence the need for air quality maintenance measures to further control particulate emissions. Note that the secondary 24-hour TSP standard is not to be exceeded more than once per year. Thus, in order for a violation of the standard to occur, the second highest 24-hour TSP concentration in a given year must exceed 150 $\mu g/m^3$. Larsen's statistical techniques were used to extrapolate such values, and the results show a predicted violation of the 24-hour standard in the Metropolitan Providence area, with values as high as 188 $\mu g/m^3$ in downtown Providence through 1985. The output from the CDM is easily used in this extrapolation, and one possible improvement to the model would be to add a Larsen subroutine to the computer code so that both annual average and 24-hour maximum concentrations could be output simultaneously.

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*The State of Rhode Island has adopted air quality standards which are identical to the NAAQS.

Thus, the modeling results indicate that further control of particulate emissions in the Metropolitan Providence AQMA will be necessary to maintain ambient air quality standards for TSP through 1985.

Evaluation of Air Quality Maintenance Strategies

The particulate control strategies tested for air quality maintenance were:

- An annual inspection and periodic maintenance program for all large industrial, commercial, and institutional boilers included in the point source inventory, including electric generating power plants
- Use of unleaded gasoline by all 1975 and newer light-duty motor vehicles included in the area source inventory.

These strategies were evaluated by making appropriate adjustments to the future projected emission inventories and then rerunning the CDM to predict future air quality. The results indicate only the use of the second strategy will maintain annual TSP levels in the AQMA below the secondary standard through 1985. Projected effects of the first strategy are to reduce future TSP levels, at most, by 1 $\mu g/m^3$.

Although predicted concentrations output by the CDM show the split between total area and total point source contributions, a detailed source-contribution file* is not produced. We consider this omission to be the principal weakness of the CDM used in this study as such data would eliminate the need to adjust emission inventories and constantly rerun the model in order to test different control strategies. By compiling source contributions at all receptor points, alternative maintenance strategies can be quickly evaluated through the application of appropriate scaling factors to only those sources affected by the strategy. Since this work was done, a version of CDM with this capability has been developed for EPA Region V.

Conclusions

The CDM was used to identify areas in the Providence AQMA where annual NAAQS for SO_2 and TSP are likely to be exceeded, and to test control strategies to maintain air quality standards. The CDM was found to be an accurate model, well suited to air quality maintenance analysis. The principal weakness of the CDM was its inability to produce a source-contribution file that would allow a more analytical approach to the evaluation of maintenance strategies. We note that subsequent to this study, a version of CDM has been developed for EPA Region V which includes this capability. The usefulness of the CDM in AQMP evaluation could also be improved upon by the addition of a Larsen subroutine to statistically extrapolate annual levels to 24-hour maximum concentrations.

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*For example, the source-contribution file produced by EPA's Implementation Planning Program.[3]

IMPROVEMENTS IN AIR QUALITY DISPLAY MODEL

Chandrika Prasad, Ph.D., P.E.
State Air Pollution Control Board
Richmond, Virginia 23219

Summary

The Air Quality Display Model (AQDM) is widely used to predict the concentration of sulfur dioxide and suspended particulates in the ambient air. This paper describes some of the difficulties encountered in the use of this model and the modifications to improve the model.

It is suggested that (1) in calibrating the model the line of the best fit be determined on the basis of the measured minus the background concentration and the calculated concentration, (2) the actual number of samples (which were used to compute the standard geometric deviation) be used in computing the highest and the second highest concentrations, (3) in computing the source contributions to a receptor the y-intercept and a part of the background not be apportioned in the individual source contribution and (4) a few modifications to the input and output formats be made. These modifications add to the usefulness of the model and the ease in reviewing the results.

Nomenclature

A = y-intercept
B = slope of the regression line
C_i = uncalibrated concentration due to source i at a receptor
C = uncalibrated total calculated concentration at a receptor
D = standard geometric deviation
E = a variable (see Appendix A)
F = plotting position frequency
G = background concentration
i = a subscript
N = number of samples
R = rank order (highest, second highest, etc.)
S_i = concentration contribution (calibrated) from source i to a receptor
S = concentration contribution (calibrated) from all sources to a receptor
T = total concentration (calibrated) at a receptor (annual arithmetic mean)
T_{max} = highest concentration (short-term)
u = uncertainty
y = measured air quality concentration
z = number of standard deviations from the mean.

Introduction

Atmospheric simulation models are frequently used to relate pollutant emissions to pollutant concentrations. Some of the models most readily available to air pollution control agencies and representative of the state-of-the-art of atmospheric simulation models are given in Reference 1.

The models estimate the concentration for a 1-hour period or for seasonal or annual averages. The long-term models such as AQDM[2*] and CDM[3] are widely used to predict the concentration of sulfur dioxide and suspended particulates. The AQDM is preferred and is the minimum acceptable[4] by the Environmental Protection Agency for air quality analysis for these two pollutants in developing the air quality maintenance plans.

The AQDM is essentially a long-term model. The model determines the impact of a variety of sources at a given receptor for a given set of meteorological conditions. It then weighs this concentration by the frequency with which that particular set of meteorological conditions occurs and then sums up over all meteorological conditions, thus producing a long-term average concentration. Basic input to the model is a comprehensive emission inventory on both point and area sources. The meteorological input to the model is a joint frequency distribution of wind speed, direction, and stability classes along with an average mixing depth.

Through a mathematic simulation of the atmospheric diffusion process, the model determines the arithmetic average of ground level concentrations over an annual period. To provide a comparison with the National Ambient Air Quality Standards the program includes a statistical model[5] which is used to relate the annual arithmetic mean to annual geometric mean and the highest concentration for a selected number of receptors.

Climatological Dispersion Model (CDM) is another long-term model frequently used. The AQDM and CDM have differences in calculation techniques; however, the two require basically the same inputs and have same types of outputs. A significant difference between the two is a source contribution table generated by the AQDM which allows the impact of each source on air quality to be evaluated. Such a source contribution table is highly desirable, especially when developing a strategy to maintain the standards. Such a table is also useful in evaluating the impact of a new source or the impact of a control program for an existing source.

Modifications To The AQDM

Several difficulties were encountered in the use of the AQDM. These are discussed in the paragraphs which follow. Also discussed are the methods to overcome these difficulties by modifying the model. These modifications cover the following areas:

- Calibration procedure, used to compute y-intercept and slope of the line of the best fit during calibration of the model
- Statistical model, used to compute annual geometric mean and highest concentration
- Source contribution table, used to generate individual source contribution to selected receptors
- Input and output formats, used for data input and results output.

Existing Calibration Procedure

Before using the AQDM to estimate regional air quality, the model is first calibrated using existing air quality data. This is accomplished by making an AQDM run using the emission, meteorological, and measured air quality data for a specific year. The calibration procedure begins with the use of the model to calculate concentration values at each of the monitor-

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[*] Numbers in superscripts denote references cited.

ing stations for which measured air quality data are available. The line of the best fit (which describes the relationship between the measured and calculated concentration) is obtained using the least-square technique. One of the following two procedures is used to handle the background concentration.

Use Of Background Concentration As Input. If an accurate value of the background concentration is available, it is included in the input data. The AQDM program adds the background concentration to the calculated concentration before attempting to determine the line of the best fit as shown in Figure 1. The regression line in this case can be described by the equation:

$$y = A + B (C + G) \qquad (1)$$

In this case, since the accurate value of the background concentration, G, was used as input, the y-intercept, A, can be considered as the unknown and might be attributed to natural sources and/or man-made sources outside the area being modeled, or it may be considered as an uncertainty due to uncertainties in the input data on emissions, meteorology, and measured air quality. For the sake of brevity, let it be called the uncertainty and denote it by 'U'. Hence, in this case, U = A.

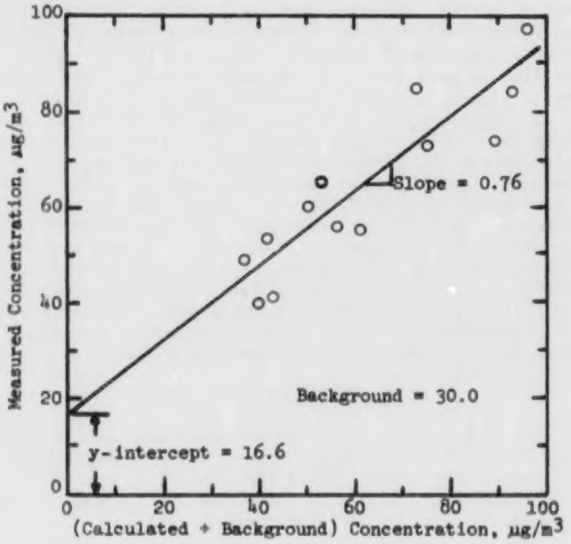

Figure 1. Regression Line (with background input)

Background Concentration Not Used As Input. If an accurate value of the background concentration is not known, it is not used in the input data. In this case the regression line is obtained by comparing the measured air quality, y, with the calculated concentration, C, as shown in Figure 2. The y-intercept in this case automatically accounts for the missing background. Thus, the y-intercept is equal to the uncertainty, U, plus the background, G . If the background is subtracted from the y-intercept, the result should be the uncertainty.

But a comparison of the results from Figures 1 and 2 (which have been drawn for the same data) indicates that the values of the uncertainties are different in these two cases. Thus we see that the two procedures are not consistent.

Modified Calibration Procedure

Since the measured air quality concentrations include the background concentration, it appears more appropriate to compare the calculated concentrations with the measured minus the background concentration as shown in Figure 3. If the background concentration is not known, it should not be used as an input; then the plot will be exactly like Figure 2. A comparison of the y-intercepts obtained from Figures 2 and 3 indicates that the difference between the two y-intercepts is equal to the background concentration.

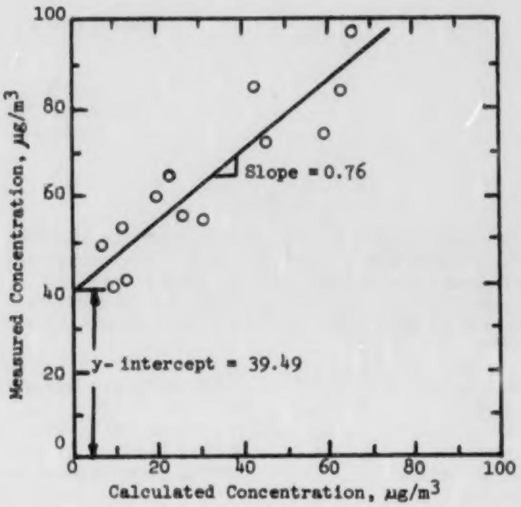

Figure 2. Regression Line (without background input)

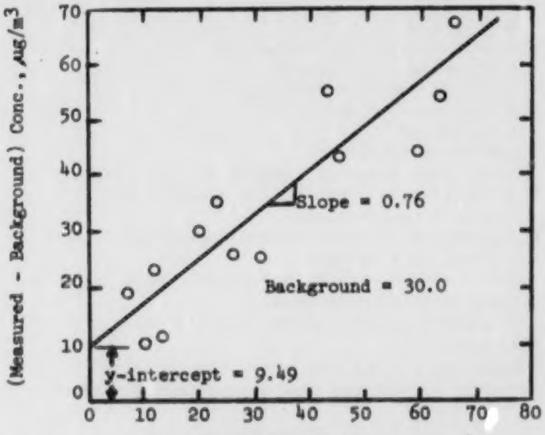

Figure 3. Modified Calibration Procedure Plot (background subtracted from measured concentration)

Thus, the determination of the line of the best fit using calculated concentration and measured minus the background concentration gives consistent results in both cases (i.e., whether background values are used in input data or not). If the background concentration is not known and hence not used as input, nothing is subtracted from the measured values, and thus, the y-inter-will consist of the background and the uncertainty; whereas if the accurate background value is known, this will be subtracted from the measured values and the y-intercept will be the uncertainty.

It is interesting to note that the slope of the regression line is the same in all three cases -

Figure 1, 2, and 3.

Computation Of Calibrated Concentration

Once the model is calibrated, the y-intercept and the slope of the regression line are used to calibrate or adjust the calculated concentrations at all the receptors. The model (without modifications) uses the following relation to compute the calibrated concentration:

$$T = A + B\ (\ C + G\ ) \qquad (2)$$

In the modified version of the program, this is done by using the relation:

$$T = A + G + B\ C \qquad (3)$$

Existing Procedure In The Statistical Model

The air quality standards for sulfur dioxide and suspended particulates are in terms of annual mean concentrations. In addition, the standards include a 24-hour value not to be exceeded more than once per year.

The AQDM program includes a statistical model to convert the annual arithmetic mean to the annual geometric mean and the highest concentration. To do this, the model requires the value of standard geometric deviations for all the receptors which are selected for the statistical output.

It should be noted that the standard geometric deviations are available only from the past historical data on measured air qualities and are available only for those receptors where there is a monitoring station. At this time there is no technique available to project standard geometric deviations for future years. At the same time, the standard geometric deviations are based on a limited number of samples, the prevalent sampling frequency being every third to every sixth day, with the sample size ranging from 60 to 120 per year. In computing the highest concentration the model assumes a sample size of 365 (continous sampling). It is further realized that to obtain 365 samples (24-hour samples) using a Hi-Vol sampler will require at least two samplers side by side. The mathematical relations used in the model to compute the highest concentrations are given in Appendix A with the only difference that the model uses the number of samples to be 365 in all cases.

If the standard geometric deviation, which is based on a limited number of samples, is assumed to be the same for continous sampling (or 365 samples) it introduces significant errors in the computed values of the highest concentrations. Figure 4 shows the ratio of the highest concentration to the annual arithmetic mean as a function of sample size for several values of the standard geometric deviation.

At the same time the model does not compute the second highest concentration which is actually desired for a comparison with the air quality standards.

Modified Procedure For The Satistical Model

It is suggested that for direct comparison with the standards, the second highest concentration be computed using the actual number of samples (which were used to compute the standard geometric deviation) for the selected receptors using the procedures given in Appendix A. Figure 5 shows the ratio of the second highest concentration to the annual arithmetic mean as a function of the number of samples for several values of the standard geometric deviations.

Existing Procedure For Source Contribution Table

The AQDM provides a table which gives the contribution from each source to each of five selected receptors. If the five receptors are not selected by the user, the program automatically selects five receptors with the highest, second, third, fourth, and fifth highest concentrations. The source contribution is given both as a concentration and a percentage of the total concentration for that receptor.

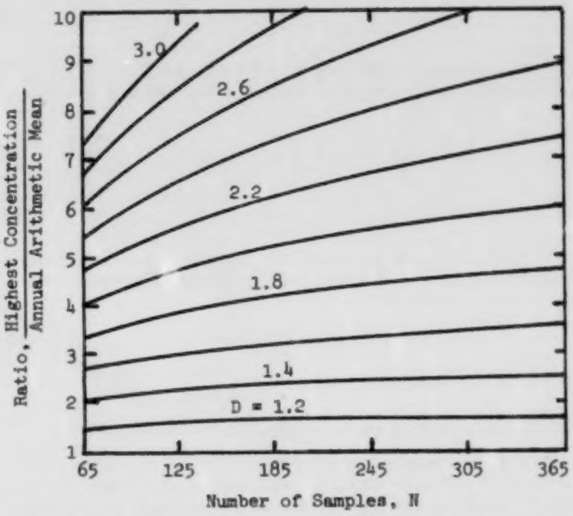

Figure 4. Ratio of the Highest Concentration to the Annual Arithmetic Mean as function of sample size and standard geometric deviation.

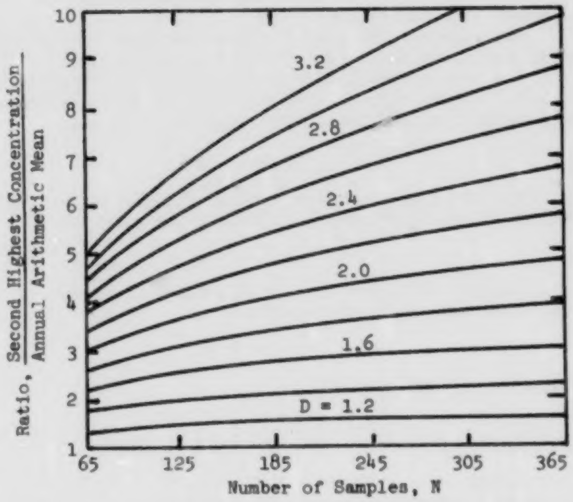

Figure 5. Ratio of the Second Highest Concentration to the Annual Arithmetic Mean as function of sample size and standard geometric deviation.

The model starts with computing the uncalibrated form of the total concentration for the specific receptor under consideration by using the following relation (which is derived from Equation 2):

$$C = \frac{T - A}{B} - G \qquad (4)$$

The model also calculates the concentration due to each source at this receptor. Let C_i be the concentration contribution due to source i to this receptor. The source contribution, S_i, due to source i to this receptor is calculated using the following relation:

$$S_i = B\,C_i + \Big[A + (B-1)\,G\Big]\frac{C_i}{C} \qquad (5)$$

The total contribution from all sources to this receptor is given by the summation of equation 5 over all sources.

$$S = \Sigma\, S_i = \Sigma\, B\,C_i + \Big[A + (B-1)\,G\Big]\frac{\Sigma\, C_i}{C} \qquad (6)$$

$$\text{or,}\quad S = B\,C + A + (B-1)\,G \qquad (7)$$

Adding the background, G, to the total source contribution, S, gives the total calibrated concentration at this receptor as

$$T = S + G = A + B\,(C + G) \qquad (8)$$

which is the same as Equation 2.

Modified Procedure For Source Contribution Table

A close examination of Equation 5 indicates that a part of the background, G, and the y-intercept, A, are apportioned in the ratio of the individual source contribution, C_i, to the total concentration, C. If there is a change in the total concentration, C, due to emissions data changes in sources other than i, the contribution from source i to the same receptor will change even though all other conditions are unchanged. This presents problems when comparing the results of one AQDM run with the other.

The procedure described below overcomes this difficulty and gives consistent results in each case.

The source contribution from source i to a given receptor should only be adjusted for the slope of the regression line and should be computed as follows:

$$S_i = B\,C_i \qquad (9)$$

The total source contribution, S, will be the summation of Equation 9 over all sources as given by

$$S = B\,C \qquad (10)$$

Adding the background, G, and the y-intercept, A, will give the total concentration

$$T = A + G + B\,C \qquad (11)$$

which is same as Equation 3.

Modifications To The Input And Output Format

Source Data. One of the basic inputs to the model is a comprehensive emission inventory on both point and area sources. The emission data for each emission point are entered on two cards. The first card (designated as SOURCE =) contains the data on source location, emission rates and stack height, as shown in Table 1. The second card (designated as PLUME =) contains stack diameter, exit gas velocity and temperature, as shown in Table 2. All the SOURCE cards are assembled together. Similarly all the PLUME cards are assembled together in the same order as the SOURCE cards, and are usually placed behind the last SOURCE card. In processing these emission data (Source and Plume Data), the Plume Data read from the first PLUME card are assigned to the first SOURCE card, the data on the second PLUME card are assigned to the data on the second SOURCE card, and so on. The model (without modifications) makes no comparison to ascertain that Plume Data are assigned to the correct Source Data.

TABLE 1. An Example Of SOURCE Data Input

	LOCATION			EMISSION (TPY)		STACK	SOURCE
	HORIZ	VERT.	AREA	SO_2	TSP	HT.	ID*
Column 10	20	30	40	50	60	70	80
SOURCE =	290.2	4243.0	0.0	53.818	2.037	122.0	'9952'
	354.3	4267.7	0.0	72.467	9.267	122.0	'9953'
	223.0	4324.6	0.0	0.000	4.247	15.0	'5701'
	223.0	4324.6	0.0	0.000	0.767	16.7	'5703'
	221.5	4312.3	0.0	12.657	38.062	58.2	'4751'
	221.5	4312.3	0.0	8.438	11.671	58.2	'4752'

* Source ID Is Additional Input Under Modified Program.

The modified program reads the source identification number entered in columns 75 to 80 of SOURCE and PLUME cards. For each point source, identical identification numbers are used on both the SOURCE and PLUME cards.

TABLE 2. An Example Of PLUME Data Input

	GAS VEL.	STACK DIA.	GAS TEMP		PLUME ID*
Column 10	20	30	40	50 - 70	80
PLUME =	12.4	5.0	392.0		'9952'
	21.6	7.9	391.0		'9953'
	53.3	4.0	419.0		'5701'
	12.5	4.0	452.0		'5703'
	12.8	4.0	401.0		'4751'
	21.5	4.3	395.0		'4752'

* Plume ID Is Additional Input Under Modified Program.

For area sources the PLUME cards are internally generated by the program. The modified program compares the source identification number with the plume identification number and if a mismatch is found, further processing of the data is stopped and the mismatch information is printed as shown in Table 3.

Sampling Station Data. Input format for the measured air quality data has been modified (as shown in Table 4) to include an identification number for data from each sampling station, and the program is modified to read these additional data. In the 'CORRELATION DATA' output these identification numbers are reprinted. At the same time, the modified program prints out calibrated concentrations. This is helpful in reviewing the Correlation Data output, an example of which is shown in Table 5.

TABLE 3. An Example Of Source Data Output

SOURCE NO.	SOURCE LOCATION (KM)		SOURCE AREA	EMISSION RATE (TON/DAY)		STACK DATA				ID NO.		
						HT.	DIA.	VEL.	TEMP.			
	HORIZ.	VERT.		SO_2	TSP	(m)	(m)	(m/s)	(^{o}K)	S*	P*	
1	290.2	4243.0	0.0	53.818	2.037	122.0	5.0	12.4	392.0	9952	9952	
2	354.3	4267.7	0.0	72.467	9.267	122.0	7.9	21.6	391.0	9953	9953	
3	223.0	4324.6	0.0	0.000	4.247	15.0	4.0	12.5	452.0	5701	5703	S/P MISMATCH
4	223.0	4324.6	0.0	0.000	0.767	16.7	4.0	53.3	419.0	5703	5701	S/P MISMATCH
5	221.5	4312.3	0.0	12.657	38.062	58.2	4.0	12.8	401.0	4751	4751	
6	221.5	4312.3	0.0	8.438	11.671	58.2	4.3	21.5	395.0	4752	4752	

* Additional output generated by the modified program.
This AQDM run was unsuccessful due to source/plume data mismatch.

TABLE 4. An Example Of SAMPLING STATION Data Input

	HORIZ. COORD.	VERT. COORD.	MEASUARD ANNUAL ARTHMETIC MEAN	STATION ID*
Column 10	20	30	40	50
PAROB =	386.0	4075.0	74.0	'176A'
	386.5	4075.1	85.0	'176D'
	384.5	4069.7	84.0	'176E'
	384.5	4071.4	97.0	'176F'
	328.0	4060.8	65.0	'178B'

* Additional Data Input Under Modified Program.

TABLE 5. An Example Of CORRELATION Data Output

SITE NO.	RECEPTOR LOCATION		PARTICULATE CONC.		ID NO. *	CALI-BRATED CONCEN. *
	HORIZ.	VERT.	OBSERVED	CALCULATED		
1	386.0	4075.0	74.0	59.0	176A	84.8
2	386.5	4075.1	85.0	43.0	176D	72.7
3	384.5	4069.7	84.0	63.0	176E	87.7
4	384.5	4071.4	97.0	66.0	176F	89.8
5	328.0	4060.8	65.0	23.0	178B	57.0

* Additional Output Generated By The Modified Program.

Source Contribution Table. The AQDM program has been modified so that all sources (point or area) contributing more than 1% to any of the five receptors are identified and their source identification numbers be printed as shown in Table 6. At the same time the maximum percentage contribution to any of the five receptors are printed. This makes the output very useful.

TABLE 6. An Example Of SOURCE CONTRIBUTION TO FIVE MAXIMUM RECEPTORS Output

SOURCE NUMBER	RECEP. 244	RECEP. 60	RECEPT. 213	RECEP. 49	RECEP. 225	ID * CODE	% * FLAG
367	0.0635	0.0470	1.3050	0.0719	0.2610		
	0.12%	0.09%	2.33%	0.14%	0.50%	1701	>2%
368	0.0361	0.0301	0.0412	0.0415	0.1118		
	0.07%	0.06%	0.07%	0.08%	0.22%	1771	
369	0.0065	0.0045	0.0196	0.0057	0.1100		
	0.01%	0.01%	0.04%	0.01%	0.21%	1801	
370	0.0022	0.0015	0.0065	0.0025	0.0373		
	0.00%	0.00%	0.01%	0.00%	0.07%	1802	
371	0.0284	0.0230	15.5964	0.0319	0.0866		
	0.05%	0.04%	27.88%	0.06%	0.17%	1811	>27%

* Additional Output Generated By The Modified Program.

Conclusions

The various modifications described above can be grouped together under the following two categories:

Modifications To The Mathematical Logics

Under this category it was suggested that

(1) During calibration of the model the line the best fit be determined by comparing the computer calculated concentrations with the measured minus the background concentration

(2) The second highest concentration be computed using the actual number of samples to compare the results with the short-term National Ambient Air Quality Standards

(3) The y-intercept and the background not be apportioned while computing the source contributions from individual sources to a receptor.

The only additional input required to carry out the modifications under this category is the data on the number of samples for those receptors which are selected for the statistical output.

Modifications To The Input And Output Formats

Under this category the additional input data required are (1) the SOURCE and PLUME identification numbers and (2) the sampling station identification numbers. These data are reproduced in the outputs on SOURCE DATA, CORRELATION DATA and SOURCE CONTRIBUTION TO FIVE RECEPTORS.

These modifications are helpful in reviewing the output results and avoid a lot of cross-referencing.

Acknowledgement

The modifications to the Input and Output formats as described previously were incorporated into the model by Erik Hougland (presently with the Tennessee Valley Authority) while working at Virginia Polytechnic Institute and State University on a contract from the Virginia State Air Pollution Control Board. His work in this area is acknowledged. The author also wishes to thank his colleague Limon E. Fortner for first pointing out the problem associated with generation of the Source Contribution Table.

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Appendix A

Computation Of Highest And Second Highest Concentration

First compute the plotting position frequency, F, using Larsen's technique[5] as given below:

$$F = 100\,\frac{R-0.4}{N} \qquad \text{(A-1)}$$

Next compute the number of standard deviations from the mean from the relations:

$$E = \left\{\ln\left(\frac{1}{F}\,2\right)\right\}^{1/2} \qquad \text{(A-2)}$$

$$Z = E - \frac{2.52 + 0.80\,E + 0.01\,E^2}{1 + 1.43\,E + 0.19\,E^2 + 0.001\,E^3} \qquad \text{(A-3)}$$

Finally, compute the highest concentration by the relation given below:

$$T_{max} = T_g\,(D)^Z \qquad \text{(A-4)}$$

where the annual geometric mean, T_g, is related to the annual aritmetic mean, T, by the relation:

$$T_g = \frac{T}{\mathrm{EXP}\,(0.5\,\ln^2 D)} \qquad \text{(A-5)}$$

In the procedure described above use R = 1 and R = 2 for computing the highest and the second highest concentrations respectively.

AIR POLLUTION MODELING IN THE DETROIT METROPOLITAN AREA

A. Greenberg
B. Cho

Air Pollution Control Division
Wayne County Department of Public Health
Detroit, Michigan

James A. Anderson, P.E.

Wayne State University and
Physical Dynamics, Inc.
Detroit, Michigan

SUMMARY

The Air Quality Display Model (AQDM) and the Climatological Dispersion Model (CDM) have been used by the Air Pollution Control Division of the Wayne County Department of Public Health and Wayne State University to simulate annual averages of suspended particulate and sulfur dioxide in the Detroit Metropolitan area. Several meteorological models including the STAR program were evaluated to determine the effect of meteorological input data on predicted concentrations. The Briggs and Holland plume rise formulas were similarly evaluated. Correlations of predicted concentrations with observations by the Wayne County Air Pollution Control Division range from .75 to above .90, depending on the combination of models used.

Applications of air pollution modeling at the Wayne County Air Pollution Control Division have dealt with developing a better understanding of how sulfur dioxide and particulate controls should be applied and in evaluating the impact of new sources on air quality. In addition, several divisions of Wayne State University are using the air pollution diffusion models in a variety of applications. The College of Engineering is developing algorithms for determining optimal air pollution control strategies with limited energy resources. The College of Lifelong Learning uses the models in an environmental simulation game called ENVIRO-ED as part of an educational effort to develop better public awareness of the environmental problems in the Detroit region. The Ethnic Studies Division of the Center for Urban Studies uses the same models for analyzing the socioeconomic impact of air pollution on Detroit area residents.

As a result of the success with the AQDM and CDM, diffusion models have become a primary tool in the Detroit area for predicting the future impact of pollutant sources on ambient air quality and for critical decisionmaking such as locating major emission sources, assessing fuel and/or process changes, locating air monitoring stations, and reviewing emission standards.

INTRODUCTION

The Detroit metropolitan area, with a population of approximately 4.7 million people, is the major industrial center of Michigan. The region consists of seven Michigan counties: Livingston, Macomb, Monroe, Oakland, St.Clair, Washtenaw, and Wayne, covering 4500 square miles and a portion of Ontario, Canada. The city of Detroit and Wayne State University are both located in Wayne County. The Air Pollution Control Division is responsible for the enforcement of applicable air pollution regulations in Wayne County which in part are designed to meet the National Ambient Air Quality Standards (NAAQS). The Division operates a basic air monitoring network of 14 continuously recording sampling stations that telemeter data back to a central processing station, plus three additional manually operated high volume air samplers. Sulfur dioxide concentrations are recorded continuously at the 14 stations and suspended particulate is measured at all 17 stations on a 24-hour sample - 6 days per week schedule. This system provided the ambient air quality data for verifying and calibrating the AQDM and CDM. Two major airports in the region are National Weather Service stations and provide local climatological data (LCD) for the meteorological needs of the models.

The 1974 emission inventory of sulfur dioxide and suspended particulate that was used in this study identified 506 point sources, 395 of which were in Wayne County. To qualify as a point source, the source must have emitted at least 5 tons per year and be part of a plant that emitted at least 25 tons per year. The remaining known emissions were included in the area source inventory.

MODEL INPUT DATA

The two major input data sets required for diffusion modeling are an emission inventory for point and area sources, and the various meteorological parameters. The sensitivity of the model to this data is such that every effort should be made to obtain the most accurate data possible.

EMISSION INVENTORY

The total inventory of emissions for the year 1974 was divided into three major categories: point sources (public utilities and major industrial, institutional, and governmental facilities); area sources (residential, commercial,and small industrial); and mobile sources (automobiles, aircraft, and vessels).

Point source emission data is determined by the amount of fuel consumed and the manufacturing process. Area source emissions are based on the fuel consumption in the residential neighborhoods, small-size domestic and commercial incinerators, and on small manufacturing processes.

Mobile source emissions primarily depend on the gasoline consumption data for passenger and commercial vehicles, but these emissions were neglected in this study because their contributions to the total mass emission rate of sulfur dioxide and suspended particulates throughout Wayne County were approximately 2% and 6%, respectively. In addition, these sources, distributed throughout the County, mathematically contribute negligible quantities at the receptor sites. We did not feel that collecting the total mobile source emissions for a grid square and placing them at some point in the grid square is a proper procedure. Rather, they should be treated as moving line sources.

Area source information was only available from Wayne County at the time. Using the UTM system, a grid of 5000-meter squares was established over Wayne County to arrive at the area source emissions. Unfortunately, our area source information was originally based on grid squares one mile in length. The layout of Detroit and Wayne County made the choice of the mile grids very logical at the time. However, grid sizes of kilometer integers are the only size acceptable to the CDM. Since 5 kilometers is very close to 3 miles, this was the smallest grid square we could use.

METEOROLOGICAL INPUT DATA

The various meteorological data such as wind speed, wind direction, sky cover, etc., were available in LCD form from the Wayne County Detroit Metropolitan Airport which is about 20 miles southwest of Detroit, or from the Detroit City Airport which is in the northeast part of the city (and Wayne County). Neither of these weather stations are in the immediate vicinity of the major pollution sources, but Metropolitan Airport seemed to provide better overall correlation and was used in most cases.

Over a period of one year, 2920 atmospheric observations are recorded at each weather station. A meteorological model then statistically calculates a joint frequency distribution of wind direction, wind speed, and atmospheric stability. The Day-Night STAR program which was developed by the National Climatic Center and is a part of the CDM, uses 16 sectors for direction, 6 classes of wind speed and 6 stability categories.(5) For the 1974 Metropolitan Airport data, this model aggregated the 2920 three-hour readings into a distribution of 153 district probabilities which were used for the CDM simulations.

A similar model developed at Wayne State University, that enables the user to aggregate the meteorological data into intervals as fine as the original data, was used to evaluate the STAR program. The LCD data was originally collected in speed intervals of 1 knot and directional intervals of 10 degrees. Using the conventional 6 stabilities, and 10 degree directional intervals, the number of distinct probabilities in the joint frequency distribution varies from 316 to 857, as shown in Table 1.

Speed Intervals (Meters per second)	Number of District Probabilities
1	857
2	582
3	448
4	372
5	316

TABLE 1. Joint Frequency Distribution

The five different distributions summarized in Table 1 were used as input to the AQDM to evaluate the usefulness of this approach. In all cases, more data are provided compared to the STAR model (which requires more computer time), but as the "fineness" of the distribution increased, the correlation of simulated versus observed data increased. These results suggest that further work is needed in this area.

Both the CDM and the AQDM used the curves of Pasquill-Gifford (4) to approximate stabilities in Detroit. The only difference between the two is the CDM uses an empirical power law to approximate the functions where the AQDM uses a table.

Four CDM computer simulations were made (Table 2). The first included only Wayne County sources in the emission inventory. We then hoped to improve the linear regression analysis in the second CDM simulation by including sources outside of Wayne County that could affect Wayne County air quality. These were few in number, but an increase in estimated concentrations at most stations of 1 to 2 micrograms per cubic meter for suspended particulate and 2 to 6 micrograms per cubic meter for sulfur dioxide was found. For CDM simulation number 3, the principal change was to increase the sulfur dioxide half-life to 3 hours. Half-life in simulations 1 and 2 were both 1.25 hours. Because of this increase in half-life, estimated sulfur dioxide concentrations increased at most stations by 3 to 6 micrograms per cubic meter.

The fourth CDM simulation used a sulfur dioxide half-life of 3 hours, but the meteorological data was representative of Detroit City Airport which is located in a residential section of Detroit, while the previous simulations all used a joint frequency distribution from Metropolitan Airport. The correlation of the regression analysis for particulate did not improve by using Detroit City Airport data, but the correlation for sulfur dioxide did improve.

PARTICULATE

Simulation	Intercept	Slope	Correlation Coefficient
1	70.4	1.06	0.70
2	67.9	1.01	0.84
3	67.9	1.01	0.84
4	61.8	1.36	0.77

SULFUR DIOXIDE

Simulation	Intercept	Slope	Correlation Coefficient
1	15.7	1.38	0.76
2	12.3	1.36	0.75
3	9.0	1.26	0.73
4	6.6	1.49	0.81

CONDITIONS

1	Wayne County Sources Only
2	All Sources In or Near County
3	Sulfur Dioxide Life of 3 Hours (previously 1.25 Hours)
4	City Airport Meteorological Data (previously Metropolitan Airport)

TABLE 2. Linear Regression Analysis of CDM Simulations

As can be seen in the table, the best correlation for particulates was simulation number 2, due to the addition of sources outside the county. For sulfur dioxide, the best correlation was achieved with simulation number 4 using a half-life of 3 hours and including sources outside the county. With a background defined by the y intercept, the high particulate background, as will be seen, is justified and understandable. The sulfur dioxide background is acceptably low in the area of only 0.003 parts per million.

CONCLUSIONS

The different simulations point out important practical aspects that must be considered when using the state of the art diffusion models for decision making purposes.

The emission inventory is extremely critical and should be arrived at very carefully. The Wayne County Air Pollution Control Division determined the point source emission inventory with data gathered principally by stack tests and emission factors (2) based on fuel consumption and the manufacturing process. A significant amount of time was devoted to the emission inventory, yet the accuracy of the suspended particulate inventory is still being questioned. Stack tests are performed under ideal conditions not always representative of day-to-day emissions. Consequently, the data supplied by industry had to be carefully scrutinized before it was used to estimate emissions. For example, collector efficiency is frequently supplied from the designer blueprints, but it is unlikely the claimed efficiency is the normal operative efficiency. Even the particulate inventory does not represent only the emission of suspended particulates, but includes varying amounts of settleable matter, dependent on the type and efficiency of the collector and the resulting size distribution of the emissions. Finally, the particulate emission inventory certainly represents only a portion of the total suspended particulate burden in the atmosphere. Much of the uninventoried suspended particulate is not the so-called natural background, but includes man-made background, i.e., suspended particulate emitted not from intended points of emission such as smoke stacks, but from wind-blown factory dust, coke piles, ventilation air, ground-up street dust from mobile sources, etc. The Wayne County Air Pollution Control Division undertook a program, sampling the ventilation air from an iron foundry and a casting plant which are considered point sources based on the quantity of emissions from their stacks. We found a greater particulate emission rate from the ventilator ducts than from the respective smoke stacks. It is mistakenly believed that except for the natural background, a conventional particulate emission inventory can account for essentially all of the atmosphere's particulate burden.

Because the man-made or unaccountable particulate background depends largely on the type of industry involved, the total particulate background (man-made plus natural) will vary across the study area. The heavy industrialized regions of Wayne County containing large power plants, iron foundries, steel mills, coke ovens, cement plants, slag piles, etc., use many processes which are dirty operations in the sense that there are many chances for the evolution of particulate matter at low heights above grade into the open air. It takes a source with excellent housekeeping practices and "total enclosure" controls to avoid these fugitive types of emissions. It is the nature of the processes in a heavy industrialized area that makes this a very difficult task to accomplish.

As the above regression analyses indicate, the CDM is doing a very acceptable job of estimating particulate concentrations. The y intercept (which is total background) is approximately 65 micrograms per cubic meter county-wide. As expected, the total background is higher in those county areas recording the heaviest suspended particulate concentrations. By taking the difference between the uncalibrated CDM estimated particulate concentrations and the measured particulate concentrations, the result is total estimated background concentrations. This is done for each receptor site. (While this may not be an exact method, it gives a feeling as to the magnitude of the unaccountable sources.) If natural background remains constant throughout the area (not too bad an assumption) the varying concentrations are due to man-made unaccounted sources. It turns out, as expected, that we can draw isopleths of total background (Figure 1).

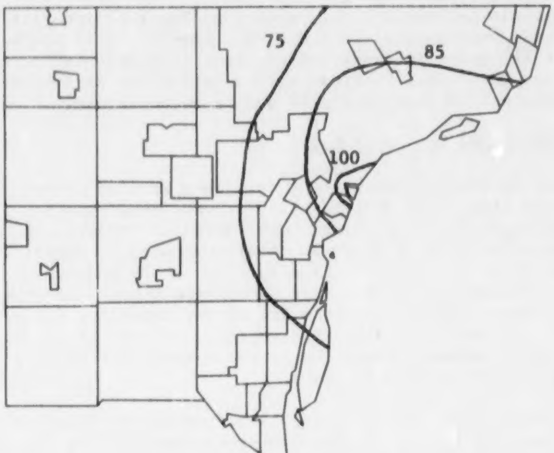

Figure 1. Total Particulate Background ($\mu g/m^3$)
Wayne County, Michigan

We find that a section of the heavy industrialized area has an annual mean background of over 100 micrograms per cubic meter. Put another way, if somehow we were able to plug up all well inventoried and intended sources of emission, the measured particulate concentrations in certain areas of the county would be well over 75 micrograms per cubic meter, the primary standard. The importance of this cannot be overstated. It relates to the practicality of ever achieving the suspended particulate NAAQS as they presently stand, and the importance of enforcement officials focusing on and paying careful attention to all possible points of emission.

In Wayne County, we have seen the importance of fugitive-type emissions on air quality as a result of a comprehensive control program at the large industrial park of the Ford Motor Company Rouge Complex. It contains basic oxygen furnaces, coke ovens, power plant, blast furnaces, large material storage piles, etc. A substantial part of the control program was to reduce or end the fugitive type of emissions attendant to a large array of processes through different types of good housekeeping practices. The once high suspended particulate concentrations measured immediately downwind of the complex and less than a quarter of a mile from the border have been reduced in two years by 30%.

CONTROL STRATEGY DEVELOPMENT APPLICATIONS

Air pollution diffusion models are also being used in the Detroit area to develop and evaluate alternative air pollution abatement strategies. The State of Michigan is a long way from being "energy independent." Estimates of the basic fuels imported to the state range as high as 95% of demand, but the state obviously has a good supply of water, which suggests that it will continue to be a major manufacturing center and perhaps even an energy converting center. As the supplies of oil and gas dwindle and prices increase, however, greater emphasis will surely be placed on using more coal, which raises at least two questions. First, would it be possible, practical, or desirable to convert many of the boilers that once burned coal back to coal? If the answer is yes, the second question is, which sources should be burning coal and how should emissions be controlled so as to reach or maintain the NAAQS in the "best" way. Many algorithms have been developed recently in an attempt to find the "optimal" solution to this problem (1). However, the existing models usually have not included fuel availability as a variable, and more importantly, the effect of a new set of fuel demands on price. Consequently, the "optimal" solution often suggests a large-scale conversion from coal to gas or oil, neither of which are in great supply. Even if the fuels were available, the new set of demands could very easily affect the prices to the point where the "optimal" solution is no longer optimal. This problem is being examined at Wayne State University by coupling an energy supply-demand model with an air pollution dispersion model similar to the AQDM. Basically, the energy model assumes that the quantity of a particular fuel available is a function of price up to the ultimate reserves of the mine or well. The model has a primary energy system that simulates the extraction of basic fuel resources and the conversion of these basic fuels to coal, oil, or natural gas. For example, coal should be converted to natural gas in the primary energy model. A secondary energy model then simulates the conversion of the basic fuels to other energy forms such as electricity and/or the transportation to the final end user, where the final energy conversion takes place. The air pollution diffusion model is used to predict the impact of all energy conversions, hence pollutant generation, on the local environment. The overall model is structured to operate in simulation or optimization mode. When the system operates in simulation mode, the air pollution model attempts to find the combination of manufacturing levels and energy end uses that will enable a set of pollution constraints, such as the NAAQS, while maximizing the net benefit to the region from energy utilization. The net benefit is defined as production profits minus the total cost of energy to the region, including industrial uses. Total cost of energy is determined by adding the cost of the basic fuels at various levels of extraction and all later conversion and transportation costs. The entire model is currently being tested on a small scale with a hypothetical community of 40,000 people. In the future, we hope to extend the model to a major metropolitan area such as Detroit.

One of the problems encountered in any project of this scope is handling the large quantities of input and output data. The AQDM and CDM models are quite satisfactory for experienced users who are dealing with a specialized air pollution problem. However, when working on a more generalized problem where air pollution is one of many constraints, such as the energy-environment dilemma, a data management system is needed to integrate those models with other simulation programs and the many sources of input data. In addition, graphic display of the simulated output data is very useful when examining regional patterns. In response to these needs, we have developed an Air Quality Information System (AQIS) that integrates the CDM, AQDM, and other related simulation models developed at Wayne State University with the U.S. Census, Census of Manufacturers, Local Climatological Data, and health data for the Detroit area. The system also includes a capability that enables the user to generate, among others, contour maps of air quality. The output from the mapping program can then be examined live on a graphic display terminal or routed to a plotter for hard copy.

EDUCATIONAL APPLICATIONS

ENVIRO-ED is a computer-assisted instruction package that deals with the involvement of the individual in problems of energy consumption, resource depletion, and environmental pollution (3). Part I of ENVIRO-ED introduces the user to air pollution, water pollution, and solid waste disposal problems and is usually the first program used. Once the individual becomes familiar with the problems, he/she is asked to clean up the air over Detroit by imposing various controls on emissions, allocating fuels, or limiting certain industrial and residential activities. Once a control strategy is identified, a simulation of air quality in the region and the control strategy costs is done with the AQIS. If the NAAQS are not met, the student is required to continue adding constraints until the standards are met. The simulation data can be displayed live on graphic display terminals such as the TEKTRONIX, but few of the users to date have had that type of hardware.

ENVIRO-ED has been used by the College of Engineering at Wayne State University with excellent success and the College of Lifelong Learning is experimenting with the programs in its new General Studies degree program.

OTHER APPLICATIONS

The Ethnic Studies Division of the Center for Urban Studies, Wayne State University, is researching the dynamics of ethnic neighborhoods in the Detroit area to identify factors causing changes in these communities and to attempt to predict future patterns. Since many of these communities originally formed near major manufacturing facilities, not too surprisingly, air pollution has always been identified as a major problem by the residents. In order to quantify the situation, the Ethnic Studies Division has used the AQIS to simulate particulate and sulfur dioxide concentrations in these ethnic neighborhoods. When these data are coupled with the 1970 U.S. Census data, they provide a cross-tabulation of pollutant concentrations with various population characteristics of Detroit, such as ethnic group, age, and income distributions.

FUTURE WORK

In the future, we plan to continue evaluating the effect of certain input data and program sub-models on the estimated concentrations of sulfur dioxide and particulate matter. We will attempt to continue updating and improving our emissions inventory with emphasis on area sources since they had a greater impact than point source emissions on selected receptor sites. Size distributions of suspended particulate and the half-life of sulfur dioxide in the Detroit area will also be investigated, which should improve the accuracy of the simulations. In addition, our efforts to evaluate alternative control strategies will receive special emphasis in case the need for large-scale conversion to coal becomes necessary in the region. The AQDM and CDM models have been found quite satisfactory for long-term simulations of sulfur dioxide and particulate. However, similar success has not been enjoyed in our efforts to model these same pollutants on a short-term basis. Consequently, we are currently developing a real-time simulation model for sulfur dioxide and particulate matter and will continue this work in the future.

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SENSITIVITY TESTS WITH A PARAMETERIZED MIXED-LAYER MODEL SUITABLE FOR AIR QUALITY SIMULATIONS

Daniel Keyser
Richard A. Anthes

The Pennsylvania State University
University Park, Pennsylvania

Summary

Several modifications to the one-layer mesoscale numerical model which Lavoie developed and applied to Great Lake snowstorms are formulated and tested. The model atmosphere consists of a parameterized constant-flux layer of fixed depth, a well-mixed layer capped by an inversion, and a deep layer of stable air overlying the mixed layer. Time-dependent calculations of the horizontal components of the wind velocity, potential temperature and the height of the base of the inversion are performed over a mesoscale grid. Since the mixed-layer assumption eliminates the dependence of the prognostic variables on height, the low-level mean flow can be predicted far more cheaply than with multi-layer models.

The major refinements introduced in this paper lie in the parameterization of the effects of the stable layer on the mixed-layer, the entrainment of mass, heat and momentum into the mixed-layer by subgrid-scale eddies, and the erosion of the inversion by heating. The sensitivity of the model solutions to the initial inversion height and strength, the stability of the upper layer, the vertical shear of the geostrophic wind, and the height of the undisturbed level in the overlying stable layer is investigated. These tests are performed for an east-west cross-section for moderate flow over complex terrain.

The Mixed-Layer Model

Multi-level primitive equation models can simulate complex, mesoscale flow patterns realistically. However, high-resolution, multi-level models require such large amounts of computer storage and time that they currently are not practical tools for everyday operational use. A simpler numerical model which requires far less computing power, but at the same time can duplicate the main results of a complicated model, would be a desirable alternative.

Since meteorologists universally recognize the importance of terrain patterns in "tuning" the local weather conditions, it is necessary to design a mesoscale model which can resolve topographic detail. Variations in surface heating and roughness also cause or "force" mesoscale circulations. Since these three effects act at the surface, one intuitively might expect them to be most important in the planetary boundary layer (PBL).

Under conditions of moderate flow or strong surface heating, the PBL can be considered well-mixed; the turbulent eddies distribute heat, moisture, and momentum uniformly in the vertical. Under such conditions, one may treat the PBL as a single layer and consider only horizontal variations in the flow. Lavoie developed a prototype mixed-layer model and applied it to mesoscale studies of Great Lake snowstorms and convective precipitation over Hawaii.[3,4] We contend that this type of model may be relevant in modeling low-level flow in more general situations.

Because the model explicitly predicts the atmosphere's behavior for the mixed-layer only, the behavior of the rest of the atmosphere must be parameterized. In the remainder of this section, we present the model and discuss its assumptions and parameterizations.

Structure of the Model Atmosphere

The lowest layer of the model consists of a thin (50m) surface layer which contains most of the wind shear and a super-adiabatic lapse rate, and follows the variable terrain (Fig. 1). The elevation of the terrain is denoted by Z_0; the height of the top of the surface layer is denoted by Z_s. The main layer extends from Z_s to the base, h, of a stable upper layer. This second layer is assumed to be well-mixed so that potential temperature, θ, and the horizontal wind velocity, V, are approximately constant in the vertical. The upper stable layer is marked by a zero or first order discontinuity in θ at its base and contains a lapse rate that is vertically constant. The winds in the stable layer are assumed to be geostrophic and may include a constant shear in the vertical.

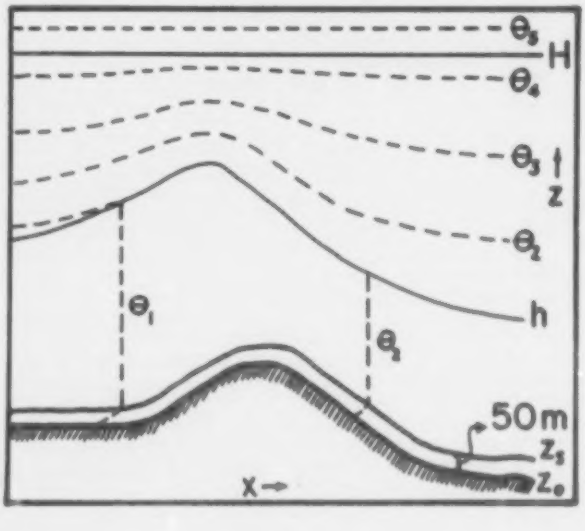

Figure 1. Hypothetical cross-section illustrating structure of mixed-layer model.

The height, h, of the mixed-layer is a material surface with the exception that subgrid-scale eddies may entrain mass, heat and momentum from the stable layer above. The entrainment depends on the surface fluxes of heat and momentum. The height, H, is the level at which the mesoscale perturbation in the potential temperature structure induced by heating or the terrain pattern is assumed to vanish.

Fig. 1 shows a cross section view of possible variations of the potential temperature structure permitted in the model. The θ_1 isentrope intersects h as a first-order discontinuity in potential temperature, while the θ_2 isentrope intersects h as a zero-order discontinuity. The vertical isentropes between h and Z_s are characteristic of a well-mixed layer. The θ-pattern between h and H indicates the response of a stable layer to a mesoscale perturbation in the PBL.

Model Equations

The derivation of the system of equations describing the physical behavior of a mixed-layer is not presented here. Instead, we present the final system of equations and discuss some of its basic properties. In order to simplify the discussion further, we only consider variations in the west to east direction. Since the vertical variations in the mixed-layer are suppressed, only horizontal variations are permitted and the model is effectively one-dimensional. The one-dimensional version retains the essential physics, but simplifies the interpretation of the results of the sensitivity tests that follow later.

Equations of motion. The partial differential equations governing the evolution of the west-east, (u), and north-south, (v), components of the horizontal wind velocity in the mixed-layer are as follows:

$$\frac{\partial u}{\partial t} = - u \frac{\partial u}{\partial x} + f \, [v - v_g(H)] + \frac{g(H - h)}{2\theta} \left[\frac{\partial \theta_h}{\partial x} - \gamma \frac{\partial h}{\partial x}\right]$$

$$- g \left[\frac{\theta_h - \theta}{\theta_h}\right] \frac{\partial h}{\partial x} + \frac{g(h - Z_s)}{2\theta} \frac{\partial \theta}{\partial x} - \frac{C_D |\underset{\sim}{V}| u}{h - Z_s}$$

$$+ K_M \frac{\partial^2 u}{\partial x^2} + \left(\frac{\partial u}{\partial t}\right)_{\text{entrainment}} \quad . \tag{1}$$

$$\frac{\partial v}{\partial t} = - u \frac{\partial v}{\partial x} - f \, [u - u_g(H)] - \frac{C_D |\underset{\sim}{V}| v}{h - Z_s}$$

$$+ K_M \frac{\partial^2 v}{\partial x^2} + \left(\frac{\partial v}{\partial t}\right)_{\text{entrainment}} \quad . \tag{2}$$

In (1) and (2), x is distance and t is time. The Coriolis parameter, f, is 10^{-4} s^{-1} and is constant in the x-direction; g is gravity, $u_g(H)$ and $v_g(H)$ are the west-east and north-south components of the geostrophic wind at the height, H; θ denotes the potential temperature in the mixed-layer; θ_h is the potential temperature in the stable layer at h, the height of the top of the mixed-layer; γ is the lapse rate of θ in the stable layer; C_D is the bulk-aerodynamic drag coefficient, and K_M is the coefficient of eddy-viscosity for horizontal momentum.

The first term on the right side of (1) is the advection of u. The second term represents the linear acceleration associated with the departure of the mixed-layer wind from the large-scale, geostrophic wind at H. The third term represents contributions to the pressure-gradient force from baroclinity and the static stability, γ, in the stable layer. The fourth term represents a restoring force associated with horizontal deformations in the height of the mixed layer. The fifth term represents the modification to the pressure gradient force due to the baroclinity of the PBL. The last three terms represent the effects of surface friction, horizontal mixing, and entrainment of u-momentum across h. The parameterized contribution of entrainment to the u-tendency is denoted by $\left(\frac{\partial u}{\partial t}\right)_{\text{entrainment}}$.

The v-equation is simpler because in the one-dimensional case north-south gradients in v, θ, θ_h, and h vanish. The mesoscale pressure gradient terms do not appear.

Thermodynamic equation. The thermodynamic equation governs the local time rate of change of θ in the boundary layer,

$$\frac{\partial \theta}{\partial t} = - u \frac{\partial \theta}{\partial x} + \frac{F_H(Z_s)}{\rho_s c_p (h - Z_s)} + K_H \frac{\partial^2 \theta}{\partial x^2} + \left(\frac{\partial \theta}{\partial t}\right)_{\text{entrainment}} \quad . \tag{3}$$

In (3) $F_H(Z_s)$ is the flux of sensible heat by eddy motions into the mixed-layer through Z_s; ρ_s is the air density at Z_s, c_p is the specific heat for dry air at constant pressure, K_H is the eddy coefficient for the horizontal transport of heat, and $\left(\frac{\partial \theta}{\partial t}\right)_{\text{entrainment}}$ represents the effect of entrainment across h. The heat flux term must be non-negative; otherwise, the mixed-layer assumption might be violated.

Mixed-layer height equation. The prognostic equation controlling the development of h is

$$\frac{\partial h}{\partial t} = - u \frac{\partial h}{\partial x} + W(h) + S \quad , \tag{4}$$

where W(h) is the vertical velocity at the height h, and S is the time rate of change of h due to entrainment of mass from the stable layer into the mixed layer.

Diagnostic equations and parameterizations. The vertical velocity is determined by neglecting local density variations and integrating the continuity equation from Z_s to h.

$$W(h) = \frac{\rho_s}{\rho_h} W(Z_s) - \left(\frac{\rho_s + \rho_h}{2\rho_h}\right) (h - Z_s) \frac{\partial u}{\partial x} \quad , \tag{5}$$

where $W(Z_s)$ is the vertical velocity at Z_s. The first term represents the effect of sloping terrain,

$$W(Z_s) = - u \frac{\partial Z_o}{\partial x} \quad . \tag{6}$$

The entrainment term, S, follows a parameterization introduced by Tennekes:[7]

$$S = \left(\frac{0.1 \, F_H(Z_s)}{\rho_s c_p} + \frac{\theta_o u_*^3}{g(h - Z_s)}\right) / \Delta\theta_i \quad , \tag{7}$$

where θ_o is the potential temperature at the earth's surface and the friction velocity, u_*, is the downward flux of momentum through Z_s. For a neutral boundary layer u_* is given by

$$u_* = C_D^{1/2} \, |\underset{\sim}{V}| \quad . \tag{8}$$

According to Deardorff[2] the inversion strength, $\Delta\theta_i$, in (7) may be defined by

$$\Delta\theta_i = \text{maximum} \begin{Bmatrix} \theta_h - \theta \\ \\ \\ 0.09(h - Z_s)\gamma \end{Bmatrix} \quad . \tag{9}$$

Equation (7) states that entrainment of mass depends on the surface heat and momentum fluxes. The entire term is modulated by $\Delta\theta_i$ which represents the resistance of the overlying stable layer to penetration by turbulent eddies.

The height of the undisturbed level, H, is arbitrarily assumed to be proportional to the depth of the perturbation induced in the h field.

$$H = h_{max} + \alpha(h_{max} - \bar{h}) \quad , \tag{10}$$

where h_{max} and $\bar{h}$ are the maximum and average values of h on the domain at a given time and α is a constant of order one.

The potential temperature lapse rate or static stability, γ, in the stable layer is given by

$$\gamma = \frac{\theta_H - \theta_h}{H - h} \quad , \tag{11}$$

where θ_H is determined by

$$\theta_H = \theta(h^i) + \gamma^i \ (H - h^i) \quad . \tag{12}$$

In (12), the superscript, i, indicates the initial value of the variable.

The geostrophic wind at H is determined by assuming the following profile:

$$\underset{\sim}{V}_g(H) = \underset{\sim}{V}_g(h^i) + \frac{\partial \underset{\sim}{V}_g}{\partial z} \ (H - h^i) \quad . \tag{13}$$

The parameters V_g and $\frac{\partial \underset{\sim}{V}_g}{\partial z}$ must be specified since they are external large-scale variables.

The effects of entrainment on the momentum and potential temperature in the PBL are calculated with the assumption of conservation of mass and enthalpy. If $\Delta h = S \ \Delta t$ is the change in the inversion height due to entrainment over a time step, Δt, then θ_h, θ, u, and v are calculated from

$$\theta_h(t + \Delta t) = \theta_h(t) + \gamma S \Delta t \tag{14}$$

$$\phi(t + \Delta t) = \frac{(h^* - Z_s) \ \phi^* + 2\Delta h \ [\phi(h^*) + \frac{\partial \phi}{\partial z} \ \Delta h]}{h^* + 2\Delta h - Z_s} \tag{15}$$

where ϕ is u, v, or θ, and an asterisk indicates the value of a variable before the effects of entrainment are considered. The factor of 2 before Δh in (15) is a consequence of using centered time-differencing.

Numerical Procedure

Time and space derivatives in the preceding equations are approximated by centered-in-time and centered-in-space finite differences. The system is integrated forward from a specified set of initial conditions over a staggered grid that is "stretched" at the boundaries. The grid increment, Δx, increases near the boundaries in order to minimize their effect on the solutions in the interior of the domain. The variables, θ, θ_h, and h are fixed at the boundaries; the velocity components are time-dependent and are determined by their values in the interior of the domain in a manner prescribed by Anthes, et al.[1] The solutions are smoothed in space and time once each hour during the integration to suppress non-linear instability.

Experimental Results

The following experiments indicate the sensitivity of the model solutions to changes in input parameters. Such information is useful if the parameter cannot be specified accurately by atmospheric measurements, or if the applicability of the parameterization is questionable.

Airflow over a Mountain

Before discussing the results of the sensitivity tests, we present a model simulation of moderate airflow over complex terrain. This case demonstrates some of the physical capabilities of the model and serves as a control experiment for the following sensitivity tests.

The experiment contains the following specifications:

$\Delta x_{min} = 20$ km

Terrain profile: smoothed west-east Appalachian profile at approximately 38°N latitude.

$C_D = 1.5 \times 10^{-3}$ over water; 7.0×10^{-3} over land

$u_g = 10 \text{ ms}^{-1}$, $v_g = 0 \text{ ms}^{-1}$, $\frac{\partial \underset{\sim}{V}_g}{\partial z} = 0$

$h^i = Z_{omax} + 500 \text{ m} = 1426.59 \text{ m}$

$\gamma^i = 5° \text{ K km}^{-1}$

$\theta^i = 290°\text{K}$, $\theta_h{}^i = 293°\text{K}$

$\rho_s = 1.21 \text{ kg m}^{-3}$ $\rho_h = 1.03 \text{ kg m}^{-3}$

No surface heating

H: $\alpha = 1$ in (10)

$$K_M = K_H = [5 \times 10^4 + 0.08 \ (\Delta x)^2 \ |\frac{\partial \underset{\sim}{V}}{\partial x}|] \ (\frac{\Delta x}{\Delta x_{min}})^2 \ [\text{m}^2 \text{ s}^{-1}]$$

The superscript, i, indicates the initial value of a variable; the subscripts max and min denote maximum and minimum values, respectively. The formulation for K_M and K_H increases the damping near the boundaries where Δx is larger than in the interior of the domain.

The initial u and v are calculated assuming a steady-state balance between frictional, Coriolis, and pressure-gradient forces. This procedure helps minimize the initial shock of starting the model.[1] For this set of specifications:

$u^i = 8.61 \text{ ms}^{-1}$ $v^i = 3.38 \text{ ms}^{-1}$ over land.
$u^i = 9.92 \text{ ms}^{-1}$ $v^i = 0.83 \text{ ms}^{-1}$ over water.

The model is integrated for 12 h using a 240 s-time step. The solutions contain transient oscillations over the integration period; these oscillations result from initial imbalances that the terrain produces in the flow. Additional experiments indicate that about 18 h of integration time are needed to attain a steady state. This adjustment time corresponds closely with the inertial period of 17.5 h associated with $f = 10^{-4} \text{ s}^{-1}$. Inertial gravity waves apparently effect the adjustment process towards a steady state; after one cycle the model variables are in balance.

We desire a quasi-steady state for the sensitivity testing because we would like to investigate the model's physical response to the fixed terrain profile with its associated surface drag, and the synoptic-scale pressure gradient force. Although the final steady-state is not reached until after about 18 h, the solutions at 12 h are quite similar to the ultimate steady-state solutions. For example, Fig. 2 depicts the 12 h and steady-state solutions of u, W(h) and h. The steady solution is the time average between 18 h and 24 h. Because of the qualitative agreement between the 12 h and steady-state solutions, the results from the sensitivity tests will be compared at 12 h.

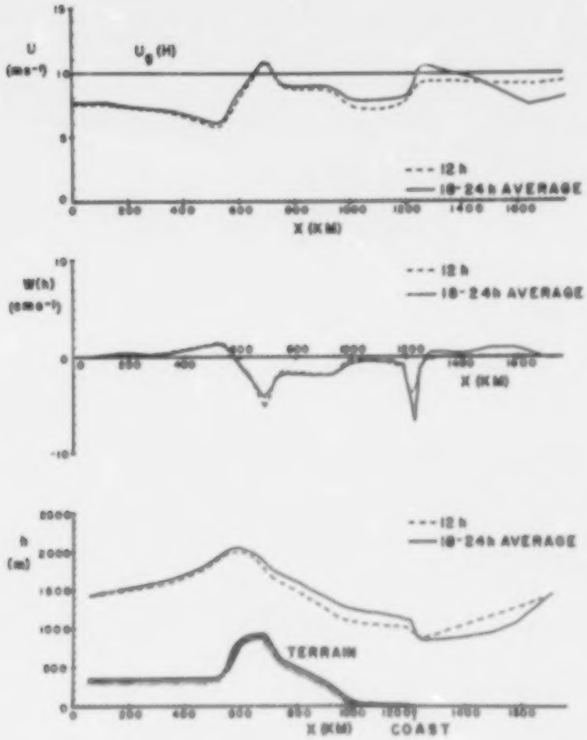

Figure 2. Profiles of u, W(h), h and terrain for the case of airflow over a mountain. The 18-24h averages represent steady-state solutions.

The 12 h u-profile shows a maximum at the ridge crest and a rapid increase at the coastline where the roughness dramatically decreases. The vertical velocity pattern shows downward motion over the ridge crest where h is a maximum. Weak upward motion occurs west of the windward slope of the mountain. The behavior of u and W(h) at the mountain ridge is reasonable in view of mountain wave structure.[6]

At the coast, differential friction causes divergence and a perturbation in W(h). The h pattern at 12 h reveals the integrated effects of the vertical velocity and entrainment. The mixed-layer height roughly parallels the terrain profile and the perturbation in W(h) has helped produce a perturbation at the coast.

Sensitivity Tests

The fields of mixed-layer height, h, at 12 h will be compared since they represent an integrated response to the velocity components and entrainment. Fig. 3 contains the results of the tests.

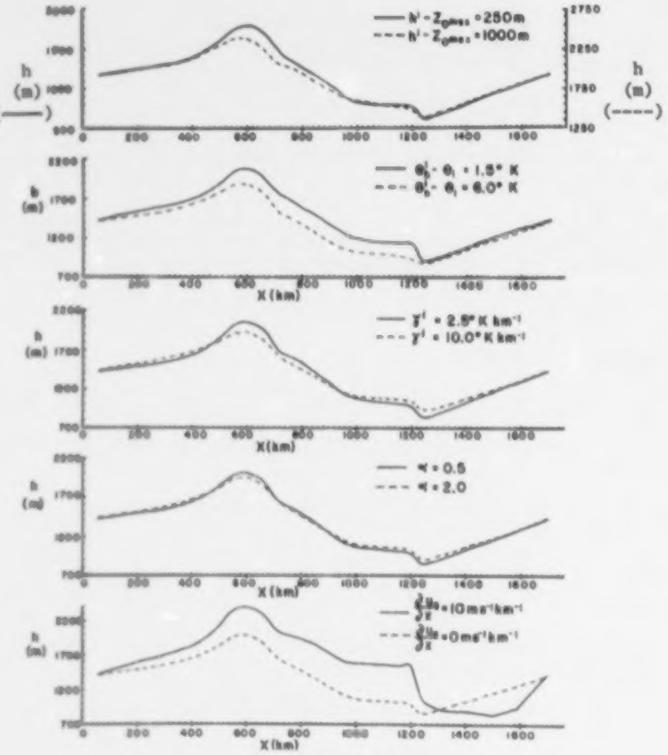

Figure 3. Sensitivity tests showing response of PBL depth, h, at 12 h to variations in the initial parameters, h^i, $\theta_h^i - \theta^i$, γ^i, α, and $\frac{\partial U_g}{\partial z}$.

Variation of h^1. Two experiments were run; one with $h^1 - Z_{omax} = 250$ m, the other with $h^1 - Z_{omax} = 1000$ m. The h curves are plotted so that their endpoints coincide despite differences in the numerical values. This presentation demonstrates their relative changes. The greatest effect of changing the initial height of the inversion occurs at the mountain, and the least variation occurs over the water. Entrainment is the factor causing the differences. In these adiabatic experiments, it is inversely proportional to the PBL depth, and is stronger over land where the roughness is greater.

Variation of initial inversion strength, $\theta_h^1 - \theta^1$.

Experiments were run for inversion strengths of 1.5°K and 6.0°K. The case with the weaker initial inversion strength shows the greater growth in h at 12 h. As in the preceding case, the changes are negligible over water where entrainment is weak. The perturbation in h at the coast is more accentuated in the less stable case $(\theta_h{}^1 - \theta^1 = 1.5°K)$.

Variation of γ^1. Experiments with $\gamma^1 = 2.5°K\ km^{-1}$ and $10.0°K\ km^{-1}$ are performed. The results indicate that for weaker γ^1, stronger perturbations in h develop at the mountain. Weaker perturbations develop when the upper layer is more stable. Qualitatively, a large restoring force from the upper layer causes weaker upward motions and less growth in h. Also, entrainment is weaker when γ^1 is large.

Variation of H. We change H by varying the parameter α in (10) from 0.5 to 2.0. At 12 h for α equal to 0.5, H equals 2330 m; for α equal to 1.0, H equals 2510 m; and for α equal to 2.0, H equals 3100 m. Increasing α by a factor of 4 increases H by about 1/3. The h fields coincide very closely, so the variations in H have little effect on the model dynamics through the restoring force. This case does not contain shear of the geostrophic wind, so $\underset{\sim}{V}_g(H)$ is independent of the value of H.

Vertical shear of u_g. In our final test we introduce a vertical shear in the geostrophic wind; $\frac{du_g}{dz}$ equal to $10\ ms^{-1}\ km^{-1}$. This value corresponds to a north-south potential temperature gradient of $-2.96°K\ (100\ km)^{-1}$ a value characteristic of frontal zones.

At 12 h the h pattern exhibits a maximum at the mountain ridge which is 500 m higher than in the case without shear. The perturbation at the coast is amplified. Including shear dramatically increases the kinetic energy in the model. The geostrophic wind, $u_g(H)$, is higher causing stronger horizontal winds and vertical velocities which intensify the perturbation in the h-field. In turn, H rises increasing $u_g(H)$. At 12 h, $H = 3096$ m and $u_g(H) = 26.7\ ms^{-1}$. The model results are reasonable for this strong a pressure gradient; however, in physically realistic experiments shears would be weaker and there would be limits on H and $u_g(H)$.

To summarize, changing h^1, $\theta_h{}^1 - \theta^1$, γ^1 and α cause relatively small differences in the model's behavior while changing $u_g(H)$ produces a significant effect. The geostrophic wind represents synoptic-scale forcing while the other parameters represent mesoscale processes. These model results indicate that in the absence of surface heating, the mesoscale motions are most sensitive to variations in synoptic-scale pressure gradients under moderate to strong wind conditions.

Application to Air Quality Simulations

Because the one-dimensional model results are encouraging, we intend to conduct further tests with diabatic heating as an additional forcing term. We then plan experiments with a two-dimensional version of the model that will utilize real data in order to determine how realistically a simple model can depict mean boundary-layer behavior.

The output of u, v, W, θ, and h can serve as input for a regional scale air quality model of a well-mixed boundary layer, where to a first approximation the concentration of a pollutant is vertically uniform. In order to maintain large horizontal gradients, particle-in-cell techniques can be used in simulating the advection of concentration patterns. If sources and sinks can be modeled realistically, reasonable estimates of pollutant concentrations should be obtainable from such a model.[5] We feel that mixed-layer models can generate the meteorological data such a model requires.

The one-dimensional mixed-layer model data can be used as input for a cross-sectional air quality model of the mixed layer. We have designed such an air quality model that considers sources, sinks and vertical diffusion on an Eulerian grid, and treats the advective transport with a particle-in-cell technique. Fig. 4 depicts the meteorological state predicted by the mixed-layer model and the associated concentration pattern of a passive contaminant in the PBL. This example demonstrates the potential of combining mixed-layer model data with a typical air quality model.

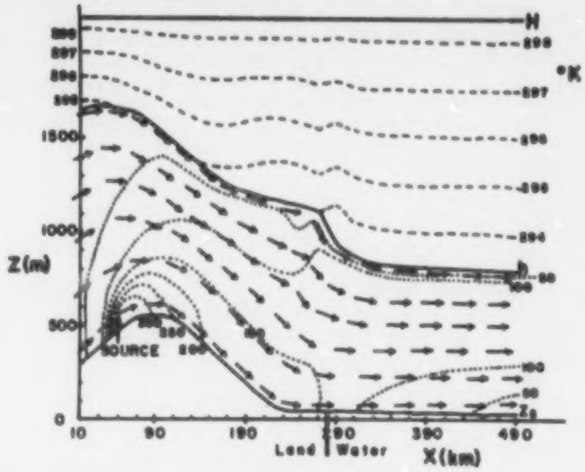

Figure 4. Cross-section depicting 12 h-mixed-layer model output and concentration of a passive contaminant derived from the air quality model. Vertical arrow at x = 50 km represents center of 20 km-wide area source of strength 35 μg m^{-2} s^{-1}. Deposition is simulated east of the coast (x > 280 km); the deposition velocity is 3 cms^{-1}. Arrows represent wind direction in the mixed-layer. Dotted lines are isopleths of contaminant concentration in units of μg m^{-3}. Dashed lines are isentropes. Potential temperature at 12 h in the mixed-layer varies from 290.55°K to 290.90°K.

Acknowledgements

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PREDICTION OF CONCENTRATION PATTERNS IN THE ATMOSPHERIC SURFACE LAYER

S. Hameed
Laboratory for Planetary Atmospheres Research
Department of Mechanics
State University of New York
Stony Brook, N. Y. 11794

S. A. Lebedeff
Institute for Space Studies
NASA, 2880 Broadway
New York, N. Y. 10025

Abstract

We present a study of turbulent diffusion in the atmospheric surface layer under conditions of neutral stability. The two-dimensional semi-empirical diffusion equation is solved using the integral method, previously described by us [3-6]. Concentration distributions at the ground are obtained for area sources and for line sources situated perpendicular to the mean wind direction. It is found that the concentration distributions are represented by simple formulas for downwind distances $x >> z_0$, where z_0 is the roughness length. Also, at such large distances, the equation for the shape of the boundary of the polluted layer obtained by the integral method is found to be the same as given by Lagrangian Similarity Theory. This equation yields the value $\lambda = 0.65$ for the ratio of the mean vertical velocity to the friction velocity in the neutral surface layer, which compares well with the value $\lambda = 0.75$ found by Kazanskii and Monin [7] from experiment.

Introduction

Prediction of pollutant concentration patterns requires solution of the diffusion equation in which the mean wind velocities and eddy diffusion coefficients appear as input quantities. In practice the mean wind velocity as a function of height is obtained from measurements while the diffusivity function is estimated with the help of a boundary layer model. Usually models of the boundary layer are based on simplifying assumptions, such as existence of steady state conditions and homogeneity in the horizontal direction, which do not correspond realistically to the urban problem where pollution dispersion is of the greatest interest. Such simplified models are, nonetheless, of interest in dispersion studies because, hopefully, they lead to an understanding of the basic processes involved. Also, methods developed for studying such simple models could be of use in the future when more realistic models of the urban boundary layer become available. In this paper we will focus our attention on perhaps the simplest dispersion problem, that is, the prediction of concentration distributions from area and line sources in the atmospheric surface layer. The surface layer is the lowest part of the planetary boundary layer in which Reynold stresses are found to be nearly constant with height. According to Monin-Obukhov similarity theory the turbulent transport processes in the surface layer are completely characterized by only two parameters, namely, the friction velocity $u_* = (\tau_0/\rho)^{1/2}$, where τ_0 is the constant value of turbulent stress and ρ is the air density, and the length scale $L = \frac{-u_*^3}{k(g/T_0)(q/C_p\rho)}$, where k is the von Karman constant, g is the gravitational acceleration, T_0 the air temperature, q the vertical heat flux and C_p is the specific heat capacity of air. In neutral conditions $q = 0$ and $|L| = \infty$; in stable conditions $q<0$ and $L>0$ and when unstable conditions prevail $q>0$ and $L<0$. In particular, the mean wind velocity $u(z)$ and the eddy diffusivity $K(z)$ can be represented in terms of a function $\phi(z/L)$ as follows:

$$\frac{\partial u(z)}{\partial z} = \frac{u_*}{kz}\,\phi(z/L),$$

$$K(z) = \frac{ku_*z}{\phi(z/L)}, \tag{1}$$

$$\phi(z/L) \rightarrow 1, \text{ as } (z/L) \rightarrow 0.$$

$$\text{Thus, } u(z) = \frac{u_*}{k}\int_{z_0}^{z}\frac{dz'}{z'}\,\phi(z'/L) = \frac{u_*}{k}\left[f\left(\frac{z}{L}\right) - f\left(\frac{z_0}{L}\right)\right] \tag{2}$$

where z_0 is the roughness length characterizing the ground roughness which is assumed to be uniform in the x,y directions. The determination of the function $\phi(z/L)$ has been the subject of several theoretical and experimental investigations [1]; in particular, Businger et al. [2] have found from observations that:

$$\phi = 1 + 4.7\,z/L \; ; \; L>0,$$

$$\text{and} \qquad \phi = \frac{1}{(1 - 15\,z/L)^{1/4}} \; ; \; L<0 \tag{3}$$

It may be noted that these forms of ϕ describe the transport of momentum in the surface layer and we assume that they are adequate also for contaminants. Equations (1-3) thus determine the wind velocity and eddy diffusivity appropriate to the surface layer for use in the diffusion equation.

The Diffusion Equation

If steady state conditions are assumed and the effect of diffusion in the x and y directions is neglected then the dispersion of an inert substance is described by the equation:

$$u(z)\,\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\,K(z)\,\frac{\partial c}{\partial z} \tag{4}$$

where $c(x,z)$ is the concentration of the contaminant and the mean wind u is taken to be along the x axis. The emission of the contaminants from a uniform, semi-infinite area source located at $z = z_0$, $x>0$ is specified by the boundary condition:

$$K(z)\,\frac{\partial c}{\partial z} = -Q \; ; \; z = z_0. \tag{5}$$

Also,

$$c(x,z) = 0 \; ; \; x = 0,$$

$$\text{and} \qquad c(x,z) = 0 \; ; \; z = \infty. \tag{6}$$

With $u(z)$ and $K(z)$ given by equations (1,2), the diffusion equation becomes:

$$\frac{1}{k^2}\left[f\left(\frac{z}{L}\right) - f\left(\frac{z_0}{L}\right)\right]\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\,\frac{z}{\phi(z/L)}\,\frac{\partial c}{\partial z} \tag{7}$$

This equation can, of course, be solved by numerical methods but we will apply an integral method to obtain its solution. We have studied application of the integral method to the diffusion equation in our previous work [3, 4, 5, 6] and we find that it is considerably simpler than numerical integration and also gives accurate solutions for the concentration distribution at the surface. In the present problem we find that the method becomes particularly simple and yields interesting results for the surface layer under conditions of neutral stability. In the following, therefore, we will solve equation (7) for the neutral surface layer; the treatment of stable and unstable surface layers is somewhat more involved and will be presented elsewhere [6].

For neutral stability $L = \infty$, $\phi(Z/L) = 1$ and $f = \log z$. Hence equation (7) becomes

$$\frac{1}{k^2} \log(z/z_o) \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} z \frac{\partial c}{\partial z} \tag{8}$$

and the boundary condition (5) reduces to:

$$k u_* z \frac{\partial c}{\partial z} = -Q \; ; \; z = z_o \tag{9}$$

Let us define dimensionless variables:

$$\xi = \frac{k^2 x}{z_o} , \zeta = \frac{z}{z_o} \text{ and } N(\xi,\zeta) = \frac{k u_* c}{Q} \tag{10}$$

Then equations (8,9) become:

$$\log \zeta \frac{\partial N}{\partial \xi} = \frac{\partial}{\partial \zeta} \zeta \frac{\partial N}{\partial \zeta} , \tag{8a}$$

$$\zeta \frac{\partial N}{\partial \zeta} = -1 \; ; \; \zeta = 1. \tag{9a}$$

In the integral method it is assumed that the distribution of the contaminant above the area source is limited to a finite depth $\zeta = \delta(\xi)$ and the contaminant concentration and its flux vanish for larger values of ζ:

$$\begin{aligned} N(\xi,\zeta) &= 0 \; , \; \zeta = \delta(\xi), \\ \frac{\partial N(\xi,\zeta)}{\partial \zeta} &= 0 \; , \; \zeta = \delta(\xi), \end{aligned} \tag{11}$$

Thus $\delta(\xi)$ represents the top of the polluted layer. We have found [5,6] that the integral method yields an accurate solution of a problem characterized by a linear diffusivity function, such as equation (8a), if we assume the solution to be of the form:

$$N(\xi,\zeta) = \eta_o(\xi)(1 - \frac{\zeta}{\delta})^2 \log (\frac{\zeta}{\delta}) \tag{12}$$

Substitution of this expression in the boundary condition, equation (9a), gives:

$$\eta_o(\xi) = - \frac{\delta^2}{(\delta-1)(\delta-1+2 \log \delta)} \tag{13}$$

Concentration at the surface $z = z_o$ is obtained by using equation (13) with equation (12) and taking $\zeta = 1$;

$$N_o(\xi,1) = \frac{(\delta-1) \log \delta}{(\delta-1+2 \log \delta)} \tag{14}$$

We now integrate the diffusion equation (8a) from $\zeta = 1$ to $\zeta = \delta$ to obtain:

$$\frac{d}{d\xi} \eta_o(\xi) \int_1^\delta (\log \zeta)(1-\frac{\zeta}{\delta})^2 \log (\frac{\zeta}{\delta}) d\zeta = \zeta \frac{\partial N}{\partial \zeta} \Bigg|_{\zeta=1}^{\zeta=\delta} = 1 \tag{15}$$

where we have used conditions (9a) and (11) on the right hand side. Integration over ξ then gives:

$$\xi = \frac{(\frac{11}{18} \delta^3 + \delta^2 - \frac{\delta}{2} + \frac{1}{9}) \log \delta - \frac{85}{54} \delta^3 + 2\delta^2 - \frac{\delta}{2} + \frac{2}{27}}{(\delta-1)(\delta-1 + 2 \log \delta)} \tag{16}$$

This is an algebraic relationship for determining $\delta(\xi)$ which together with equation (14) gives the concentration distribution at $z = z_o$.

With reference to the definitions (10) we note that δ has been expressed in units of z_o. Since z_o is usually small (~1 cm) we have $\delta >> 1$, except in a small region very close to the upwind edge of the area source. Hence we may use the approximation

$$\xi \simeq \frac{11}{18} \delta \log \delta - \frac{85}{54} \delta \; ; \; \delta >> 1 \tag{17}$$

and replace equation (14) by:

$$N_o(\xi,1) \simeq \log \delta \; ; \; \delta >> 1. \tag{14a}$$

The increase in the depth of the pollutant cloud with distance according to equation (16) is compared with the approximation (17) in Fig. 1, and the corresponding increase in the surface concentration over an area source $N_o(\xi,1)$, according to equations (14) and (14a) is shown in Figure 2. It may be noted that this solution is for a uniform area source which extends from $x = 0$ to $x = \infty$. Concentration distributions for sources of finite extent or spatially varying emission strengths can be constructed from this basic solution by superposition, as shown in [3,6]. Furthermore, if $M(\xi,\zeta)$ is the concentration distribution due to an infinitely long line source situated at right angles to the mean wind direction, then, as explained in [6],

$$M_o(\xi,1) = \frac{d}{dx} N_o(\xi,1) = \frac{k^2}{z_o} \frac{dN_o}{d\xi} \tag{18}$$

We differentiate equation (14) and consider the case $\delta >> 1$ and obtain:

$$\begin{aligned} M_o(\xi,1) &= \frac{k^2}{z_o} \frac{1}{\delta} \frac{d\delta}{d\xi} \\ &= \frac{k^2}{z_o} \frac{1}{(\xi + \frac{11}{18} \delta)} \end{aligned} \tag{19}$$

This result is shown as the dash-dot curve in Fig. (2).

Shape of the Contaminated Layer

Calculation of the shape of the boundary of the contaminated layer due to a source located on the ground has been the subject of several investigations on the basis of the Lagrangian Similarity Theory [1]. Also, Kazanskii and Monin [7] have experimentally observed the dispersion of smoke from a maintained line source in the surface layer in near-neutral conditions. They have explained the observed shape by arguing that, since the friction velocity u_* is the only velocity scale in the surface layer, the mean vertical velocity of particles at the top of the contaminated layer should be:

$$\frac{d\tilde{Z}}{dt} = \lambda u_* \tag{20}$$

where $\tilde{Z}$ represents the top of the layer and λ is a constant. Also, neglecting the effect of horizontal diffusion, the smoke particles may be taken to move along the horizontal direction with the mean velocity of the wind:

$$\frac{dx}{dt} = u(\tilde{Z}) = \frac{u_*}{k} \log (\frac{\tilde{Z}}{z_o}) \tag{21}$$

Thus, combining equations (20,21) one obtains for the shape of the boundary:

$$\frac{dx}{d\tilde{Z}} = \frac{1}{\lambda k} \log (\frac{\tilde{Z}}{z_o}) \tag{22}$$

In the integral method used in the previous section, the shape of the boundary is given by equation (16) which yields for $\delta >> 1$:

$$\frac{d\xi}{d\delta} = \frac{11}{18} \log \delta - \frac{26}{27} . \tag{23}$$

With reference to the definitions (10), writing $\delta = \frac{\tilde{Z}}{z_o}$, and neglecting the constant term asymptotically, equation (23) becomes:

$$\frac{dx}{d\tilde{Z}} = \frac{11}{18k^2} \log (\frac{\tilde{Z}}{z_o}) \tag{24}$$

which on comparison with equation (22) shows that the shape of the pollutant layer obtained by the integral method is in essential agreement with that obtained by Lagrangian similarity arguments in the region suffi-

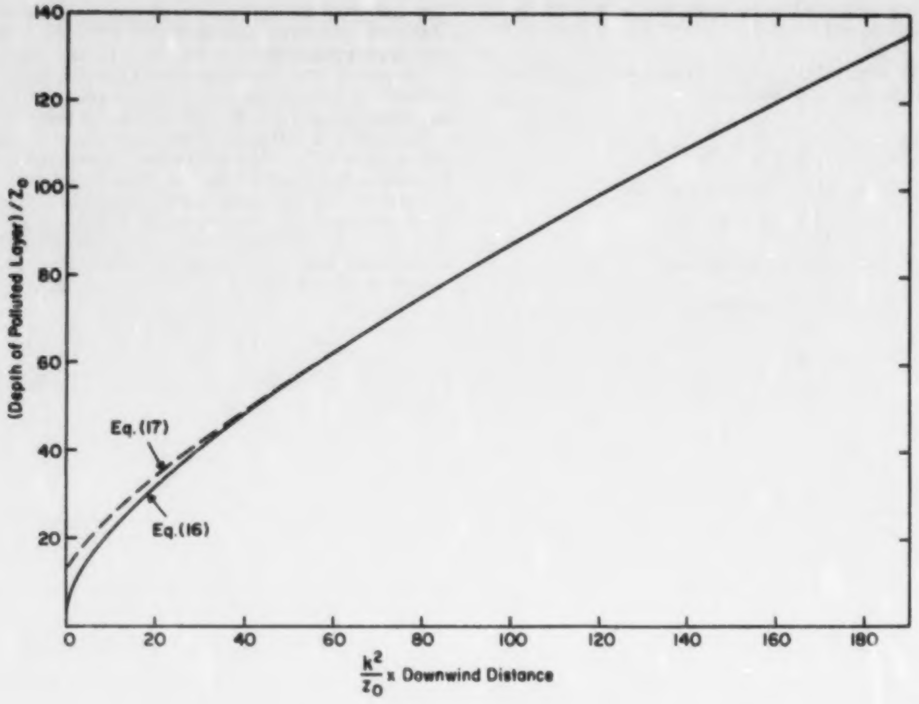

Figure 1. Variation of the depth δ with the downwind distance . The error in equation (17) is 1.6 percent at δ = 100.

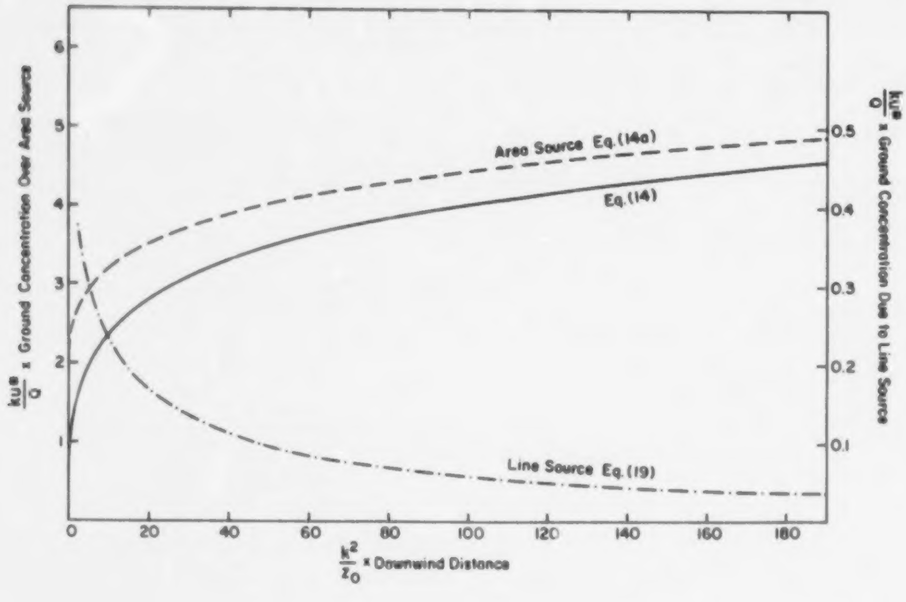

Figure 2. Variation of ground level concentation with the downwind distance ξ. —— Area Source, equation (14). ---- Area Source, equation (14a). -·-·-·- Line Source, equation (19). The error in equation (14a) is nearly 10 percent at ξ = 100.

ciently removed from the upwind edge of the source. If the right hand sides of equations (22,24) are equated we obtain:

$$\lambda = \frac{18k}{11} = 0.65 \qquad (25)$$

which may be compared with the value $\lambda = 0.75$ obtained by Kazanskii and Monin from estimates of u_* and $(d\tilde{Z}/dt)$ in their experiments. Considering the necessarily ambiguous definition of the top of the contaminated layer this agreement is encouraging because it shows the essential validity of the integral method.

Conclusions

We have analyzed the dispersion process in the atmospheric surface layer under steady state conditions. By applying the integral method to the case of neutral stability we find that for a semi-infinite area source the concentration distribution at the surface $z = z_0$ is given by:

$$c_A(x,z_0) = \frac{Q}{ku_*} \log\left(\frac{\tilde{Z}}{z_0}\right)$$

where

$$\frac{11}{18}\tilde{Z} \log\left(\frac{\tilde{Z}}{z_0}\right) - \frac{85}{54}\tilde{Z} = k^2 x$$

in the region $\tilde{Z} >> z_0$. For an infinite line source perpendicular to the mean wind the method gives

$$c_L(x,z_0) = \frac{Q}{ku_*} \frac{1}{x + \frac{11}{18k^2}\tilde{Z}} .$$

In the asymptotic region $\tilde{Z} >> z_0$ we find that the equation of the top boundary of the contaminated layer is given by

$$\frac{dx}{d\tilde{Z}} = \frac{11}{18k^2} \log\left(\frac{\tilde{Z}}{z_0}\right)$$

which when compared with the corresponding equation (22) obtained from Lagrangian similarity arguments gives $\lambda = 0.65$ for the constant of proportionality between the mean vertical velocity in the neutral surface layer and the friction velocity.

Acknowledgement

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A TIME DEPENDENT, FINITE GAUSSIAN LINE SOURCE MODEL

John C. Burr
Environmental Evaluation Section Chief
Ohio EPA
Columbus, Ohio

Robert G. Duffy
Water Quality Surveillance Section Chief
Ohio EPA
Columbus, Ohio

Introduction

Mathematical models of atmospheric diffusion range between two extremes. On the one hand there exist models which depend upon the facility with which computers are able to crunch numbers. In some situations they are the only means of obtaining a worthy answer. However, cause and effect are difficult to trace.

On the other hand are models which rely upon simplifying assumptions to yield a closed-form solution. These solutions represent a limited number of turbulent conditions. To extend their applicability, ad hoc assumptions are often introduced to represent additional conditions.

The model presented here lies somewhere between these extremes. It expresses the concentration in terms of the more readily observed physical parameters and does so in a realistic and continuous manner. The dispersion sub-model further extends the model to explicitly incorporate mechanical and thermal turbulence.

The Field Equations

The field equation for concentration ζ of a conservative material at a point in a flow of uniform velocity u is

$$\frac{\partial\zeta}{\partial t} + u\partial\zeta/\partial x = \frac{\partial}{\partial x}(K_1\partial\zeta/\partial x) + \frac{\partial}{\partial y}(K_2\partial\zeta/\partial y) + \frac{\partial}{\partial z}(K_3\partial\zeta/\partial z) \tag{1}$$

The speed u is parallel to the x axis, z is the vertical axis, and the transfer coefficients in each direction are represented by K_1, K_2, K_3. In general

$$K \sim K(x,y,z,t).$$

Looking toward the dispersion sub-model, we adopt a representation which satisfied Taylor's Hypothesis.[1] That is, for times, t, which are small compared to the Lagrangian time scale of the diffusion process, the rms dispersion $\hat{z}$ is given by $\hat{z} = at$, where a is the dispersion speed. We then represent the transfer coefficients by $K_i = a_i\sigma_i$, where σ_i is the instantaneous scale of dispersion.

We now assume that a is invariant in space and time, i.e., $a_i\sigma_i = a^2{}_i t$ and solve equation (1) for the boundary conditions $\zeta(x - ut, y, z, t^2/2) = \delta(x - ut, y, z, t^2/2)$ where δ is the Dirac delta function, whence

$$\zeta = \frac{(\sqrt{2\pi}t)^{-3}}{a_1a_2a_3} \exp - \{(x - ut)^2/2a_1{}^2t^2 + y^2/2a_2{}^2t^2 + z^2/2a_3{}^2t^2\} \tag{2}$$

This equation represents the concentration due to an instantaneous release at t = 0, x = 0, y = 0, z = 0 for fixed dispersion speeds. It may be integrated in closed form for various conditions of interest. Two of these, the unsteady plume, and the infinite, unsteady line source have been dealt with by Lissaman.[2]

The Unsteady Line Source

Consider a temporally varying line source (Figure 1) of strength Q(t), and length L, oriented at an angle ϕ to the x-axis, with $\vec{u}$, as before, parallel to the x-axis. A receptor located at (x,y) has coordinates $(x - \xi\cos\phi,\ y - \xi\sin\phi)$ relative to an arbitrary point (ξ,ϕ) of the source. At the point (x,y,z) the concentration for a time period $T = T_2 - T_1$, may be written

$$\zeta(x,y,z,T) \equiv C_L(x,y,z,T)/Q(T) \tag{3}$$

$$= \int_{T_1}^{T_2}\int_0^L \zeta(x - ut - \xi\cos\phi,\ y - \xi\sin\phi,\ z,t)\,d\xi\,dt$$

for a constant emission rate, Q(T) over the period T. After introduction of the explicit form of $\zeta(x,y,z,t)$ from equation (2), equation (3) may be integrated to yield

$$\zeta(d,\ell,z,T) = (4a_ha_vr\sqrt{2\pi})^{-1}\exp - \left(\frac{z^2u^2\sin^2\phi}{2a_h{}^2a_v{}^2r^2}\right)$$

$$\times\Big[\mathrm{erf}(2^{-\frac{1}{2}}[(d/a_h{}^2r)u\sin\phi - r/T_2])\times$$

$$(\mathrm{erf}(2^{-\frac{1}{2}}a_h^{-1}[u\cos\phi + (L-\ell)/T_2]) - \mathrm{erf}(2^{-\frac{1}{2}}a_h^{-1}[u\cos\phi - \ell/T_2]))$$

$$- \mathrm{erf}(2^{-\frac{1}{2}}[(d/a_h{}^2r)u\sin\phi - r/T_1])\times \tag{4}$$

$$(\mathrm{erf}(2^{-\frac{1}{2}}a_h^{-1}[u\cos\phi + (L-\ell)/T_1]) - \mathrm{erf}(2^{-\frac{1}{2}}a_h^{-1}[u\cos\phi - \ell/T_1]))\Big]$$

where $a_h \equiv a_1 = a_2$, $a_v \equiv a_3$ and x,y have been transformed to the source coordinates:

$$d = x\sin\phi - y\cos\phi,\quad \ell = x\cos\phi + y\sin\phi,$$

with $$r^2 = z^2/a_v{}^2 + d^2/a_h{}^2$$

and where $\mathrm{erf}(X) = \sqrt{4\pi}\int_0^X \exp(-x^2)dx$.

Note that $\mathrm{erf}(-X) = -\mathrm{erf}(X)$. Substitution of L/a_2 for L/a_h, u/a_1 for u/a_h, $[(x/a_1)\sin\phi - (y/a_2)\cos\phi)]$ for d/a_h, and $[(x/a_1)\cos\phi + (y/a_2)\sin\phi)]$ for ℓ/a_h, removes the restriction that $a_1 = a_2$.

Characteristics

The solution appears rather complicated. However, when one notes that certain combinations of variables appear more than once, it doesn't seem quite so formidable.

One is tempted to simplify the equation by taking the limit as T_1 approaches zero. However, this produces a discontinuity at $\ell = 0$, L although it yields solutions having the proper form when $0 < \ell < L$ or for ℓ outside this range. The difficulty arises when one attempts to evaluate terms such as $\lim\{\ell/T\}$

as ℓ and T both approach zero because there is no "right" way to evaluate the limit. For this reason we recommend retaining T_1 finite, though small.

In order to gain some insight into this solution it is helpful to examine how it represents various limiting cases such as: symmetric conditions; parallel, perpendicular, and zero wind; infinite line source ($L, \ell \rightarrow \infty$); and steady state ($T_2 \rightarrow \infty$) conditions. For ease of examining these cases we'll work with the form in which $T_1 \rightarrow 0$ and restrict the receptor to the range $0 < \ell < L$:

$$\zeta(d,\ell,z,T) = (4a_h a_v r\sqrt{2\pi})^{-1}\exp - \{\frac{z^2u^2\sin^2 \phi}{2a_h{}^2 a_v{}^2 r^2}\}$$

$$x(2 + \mathrm{erf}\{2^{-\frac{1}{2}}[(d/a_h{}^2 r)u \sin \phi - r/T]\}) \tag{5}$$

$$x\left[\mathrm{erf}\{2^{-\frac{1}{2}}a_h{}^{-1}[u \cos \phi + (L-\ell)/T]\} - \mathrm{erf}\{2^{-\frac{1}{2}}[u \cos \phi - \ell/T]\}\right])$$

Wind Vector

A most satisfying feature of this model is that the expression retains its significance as the wind vector approaches zero; that is, as u and/or ϕ approach zero. The terms $u \sin \phi$ and $u \cos \phi$ represent the perpendicular and parallel components of the wind respectively. When the wind is perpendicular ($\phi = 90°$) to the line source the third term reduces to:

$$[\mathrm{erf}\{2^{-\frac{1}{2}}a_h{}^{-1}(L - \ell)/T\} + \mathrm{erf}\{2^{-\frac{1}{2}}a_h{}^{-1}\ell/T\}] \tag{6}$$

The concentration is symmetric about $\ell = L/2$ as may be seen by substituting $\ell = L/2 \pm \Delta\ell$. It is a maximum at the midpoint, and decreases toward either end.

If the source may be considered to have infinite extent, i.e., $\ell/(\sqrt{2}a_h T) \gtrsim 4$, this term reduces to a value of 2. Thus for an infinite source with perpendicular wind, equation (6) reduces to:

$$\zeta = (2a_h a_v r\sqrt{2\pi})^{-1}\exp - \{\frac{z^2u^2}{2a_h{}^2 a_v{}^2 r^2}\} \tag{7}$$

$$X\left[1 + \mathrm{erf}\{2^{-\frac{1}{2}}[a_h{}^{-2}du/r - r/T]\}\right]$$

which agrees with the expression derived by Lissaman.[1]

When the wind is parallel to the source the second term reduces to $2 - \mathrm{erf}\{2^{-\frac{1}{2}}r/T\}$. This term represents the process whereby the emitted "cloud" diffuses to a receptor located at a distance d from the source with no advection occurring.

The zero-wind speed solution is seen to be:

$$\zeta = (4a_h a_v r\sqrt{2\pi})^{-1}[2 - \mathrm{erf}\{2^{-\frac{1}{2}}r/T\}] \tag{8}$$

$$X[\mathrm{erf}\{2^{-\frac{1}{2}}(L - \ell)/a_h T\} + \mathrm{erf}\{2^{-\frac{1}{2}} /a_h T\}]$$

with the entire, foregoing discussion about symmetry, diffusion, and advection being applicable.

Time

Subject to the initial restriction regarding Lagrangian time scales, and a periodically steady source, the model provides a realistic representation of temporal effects. A very important benefit of the explicit representation of time in this model is the elimination of the question of what sampling time is represented by the model.

Equation (5) yields a steady-state solution

$$\zeta = (2a_h a_v r\sqrt{2\pi})^{-1}\exp - \{\frac{z^2u^2\sin^2\phi}{2a_h{}^2 a_v{}^2 r^2}\} \tag{9}$$

The infinite source, steady-state solution, (c.f. Equation (6)), on the other hand is:

$$\zeta = (2a_h a_v r\sqrt{2\pi})^{-1}\exp - \{\frac{z^2u^2\sin^2\text{[illegible]}}{2a_h{}^2 a_v{}^2 r\text{[illegible]}}$$

$$X[1 + \mathrm{erf}\{2^{-\frac{1}{2}}(d/a_h{}^2 r)u \sin \phi\}] \tag{10}$$

Both equation (9) and (10) are independent of source extent which, in fact, they should be. The two different forms illustrate the problem of taking simultaneous limits of time and geometry.

The approach to a steady-state solution in the special cases of perpendicular, parallel, and zero wind may be inferred from the previous discussion. In all cases the concentration increases as the steady-state is approached.

Dispersion Relations

The dispersion speeds are evaluated from the Monin-Obukhov[3] similarity theory of turbulence in the lower boundary layer of the earth. This model states that a steady self-similar two-dimensional boundary layer can be described by ground roughness, z_0, temperature, T, and the height invariant heat and momentum fluxes. These fluxes are characterized by u*, the friction velocity, and H, the convective heat flux. The Monin-Obukhov scale length is defined by

$$L = -u^{*3}\rho CpT/kgH$$

where ρ is the density, Cp is the specific heat at constant pressure, k is von Karmans constant, and g is the gravitational constant. Both turbulent and mean speeds are expressible as $u/u^* = f(z/z_0, z/L)$ where the form of f is a function of the type of velocity. Lumley and Panofsky[4] express the mean horizontal speed as:

$$u = u^*[\ln z/zo - \psi(z/L)]/k \tag{11}$$

where ψ, the non-adiabatic part of the profile is plotted in reference 4.

According to the theory, the vertical fluctuation velocity, a_v, is given by an equation of the form $a_v = u^*F(Z/L)$. Panofsky and McCormick[5] postulated that a_v should be a function of height, z, the rate of energy supply by mechanical turbulence,

$$\varepsilon_1 = u^{*2}\partial u/\partial z$$

and the rate of supply of convective energy

$$\varepsilon_2 = gH/\rho CpT.$$

They derive an expression for a_v which may be written as

$$a_v = 1.05(u^{*3}S/k + 2.4\ zgH/\rho CpT)^{1/3} \qquad (12)$$

where S, the wind shear, is given by $S = (kz/u^*)\partial u/\partial z$.

The effect of the convective heat flux, H, on the dispersion speed is much smaller than the effect of the wind speed and, consequently it doesn't require as great preceision in its determination. Measured values of H may be used, or, near the ground, it may be estimated from temperature and insolation data.

The wind shear, S, may be derived from measurements of the variation of wind speed along the vertical axis. In the more common case where S is not known, additional relationships are needed among S, L, and ψ in order to fit the observed wind speed by means of equation (11) and subsequently to solve for a_v from equation (12). We make use of Ellison's[6] interpolation equation

$$S^4 - 18(z/L)S^3 = 1 \qquad (13)$$

and, by taking[4]

$$\psi(z/L) = \int_{z/L}^{0} [1 - S(\xi)]d\xi/\xi \qquad (14)$$

By solving for ξ and $d\xi$ from equation (13) and using partial fractions the integral may be evaluated in closed form. Equation (13) is solved for S by use of a Maclaurin series expansion for values of S near the origin, and by two iteration forms for z/L positive or negative. They converge in five or six cycles.

Ellison's interpolation equation represents well the wind shear for unstable, neutral, and slightly stable conditions. However, neither it nor any other equation known to the authors does a good job of representing more stable conditions. Therefore this model should be used in stable cases with caution.

Temporal Effects

Since the model contains an explicit representation of time one would hope to be able to describe the effect of step changes in emission rate, wind vector, and dispersion speed. Important temporal changes immediately come to mind such as varying vehicle speeds and/or varying vehicle-to-capacity ratios. Another important practical condition occurs when pollution is caused to shift back and forth across a receptor under light and variable wind conditions.

The principal problem of describing these effects is that of either (a) representing the change in the concentration after the step change of a variable or (b) matching concentrations at the time of a step change of a variable.

We wish to consider the representation of concentration produced by step changes in the emission rate, Q, the wind, u, and the dispersion speed, a. Thus

$$C(u,a,T) = \Sigma Q_i \zeta(u_i,\ a_i,\ T_i)$$

will be the general expression for the concentration at time T.

Change of Emission Rate

Imagine that a source operating under conditions u_1, a_1, undergoes a step change in emission rate from Q_1 for times $T < T_1$ to Q_2 for times $T > T_1$. The concentration at time $T > T_1$ may be calculated by adding a differential source, of emission rate $(Q_2 - Q_1)$, which commences at time T_1, to the continuing, old source:

$$C(u,a,T) = Q_1\zeta(u_1,a_1,T) + (Q_2 - Q_1)\zeta(u_1,a_1,T - T_1).$$

For T sufficiently large, $\zeta(u,a,T - T_1)$ becomes equal to $\zeta(u,a,T)$ so that if $Q_2 = 0$, the concentration eventually decays to zero.

Wind Change

The wind, u, or its components $u \sin \phi$ along d, and $u \cos \phi$ along L, in equation (4) acts merely to transport (advect) the pollutant from the source to the receptor located at (d,ℓ,z). Imagine that a source operating at a rate Q_1 with dispersion speed a_1, is subject to a step change of wind from u_1 at times $T < T_1$ to u_2 at times $T > T_1$. Since the wind acts only to transport the pollutant all we need do is describe how the wind changes from u_1 to u_2 at times $T >> T_1$. This is given by:

$$\hat{u} \equiv u(T > T_1) = u_2 + (u_2 - u_1)T_1/T.$$

Thus, if the wind undergoes a step change from u_1 at times $T < T_1$ to u_2 at times $T > T_1$, the concentration at any time $T > T_1$ becomes:

$$C(u,a,T) = Q_1\zeta(\hat{u},a_1,T).$$

This is equivalent to what Lissaman[2] calls the ". . . standard solution for a moving receptor . . . .".

If the emission rate also changes from Q_1 at times $T < T_1$ to Q_2 at times $T > T_1$ one again adds a differential source, of emission rate $(Q_2 - Q_1)$, which commences at time T_1 but which now is subject to a wind u_2. In this case the concentration at time $T > T_1$ is given by

$$C(u,a,T) = Q_1\zeta(\hat{u},a_1,T) + (Q_2 - Q_1)\zeta(u_2,a_1,T - T_1).$$

Change of Dispersion Speed

The foregoing are exact solutions for the concentration existing at times $T > T_1$ when, at $T = T_1$, the emission rate changes from Q_1 to Q_2 and/or the wind changes from u_1 to u_2. It is not clear that changes in the dispersion speed, a, may be treated exactly.

Physically the dispersion speed serves to specify, as a function of time, the distance of a "labeled" parcel of the dispersing "cloud" from an observer moving with the "cloud". Thus, a reasonable approximation would appear to be to treat step changes in the dispersion speed, a, in the same manner as step changes in wind speed are treated. Thus if a source, operating at a rate Q_1 under a wind u_1, is subject to a step change from a_1 for times $T < T_1$ to a_2 at times $T > T_1$, define:

$$\hat{a} \equiv a(T > T_1) = a_2 + (a_2 - a_1)T_1/T,$$

then the concentration at any time $T > T_1$ becomes:

$$C(u,a,T) = Q_1\zeta(u_1,\hat{a},T)$$

Within the constructs outlined here the effect of combinations of step changes in emission rate, dispersion speed, or wind may be calculated.

Validation

We have not had the opportunity to validate the model. However, Panofsky and McCormick[5] present validation data for the dispersion speed sub-model. Lissaman[2] found that concentrations of carbon monoxide predicted by the infinite line source model correlated well with measured concentrations without any adjustment of the predicted values.

Conclusions

A reasonably simple, closed-form model of the finite line source has been found. The model produces finite solutions in a continuous manner for the limiting conditions of steady-state, infinite source, and zero-wind. It predicts reasonable concentrations at any point relative to the source. The entire model, including the dispersion relation, incorporates the important parameters of wind, surface roughness, and heat flux in a rational manner. It can be extended to model unsteady conditions. The simple analytical form of the model makes it suitable for construction of network roadway models.

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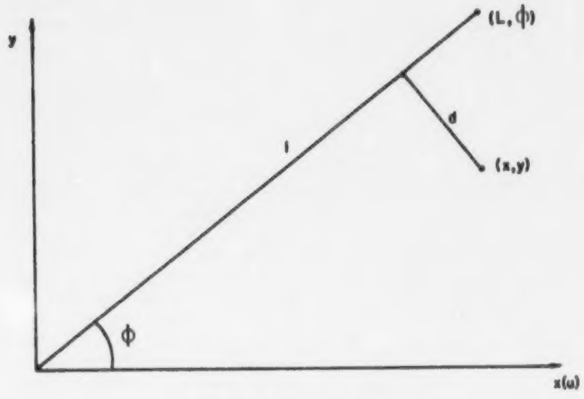
Figure 1



Source-Wind-Receptor Geometry

WATER QUALITY MODELING IN TEXAS

Joseph J. Beal, P.E.; Andrew P. Covar; and Dale W. White, P.E.
Engineering Analysis and Modeling Section
Texas Water Quality Board
Austin, Texas

Abstract

The State of Texas, acting through the Texas Water Quality Board, has been intensely interested in water quality modeling for the last three years. In the past, this effort has dealt mainly with the waste load evaluation program, made necessary for the allocation of point source waste discharges by Public Law 92-500. A considerable amount of water quality modeling will be required for the evaluation of treatment alternatives which will be developed under Section 208 of the same law. This modeling effort will consider the effects of point and nonpoint waste sources on receiving water quality, both under steady-state and time variable conditions.

Introduction

As far back as 1968, mathematical modeling studies in the State of Texas were being conducted to determine how much to restrict the discharge of pollutants. Dissolved oxygen is the parameter most often evaluated by our modeling studies. Other parameters ranging in difficulty from conservative substances to eutrophication processes have been studied. The objective of this paper is to show how applied models are used in planning problems and water quality management decisions in the State of Texas. The various types of models currently in use are discussed along with the State's future need for models.

The Role of Modeling in Water Quality Management Prior to Public Law 92-500

Prior to Public Law 92-500, the Texas Water Quality Act was the basic legal authority for the Texas Water Quality Board's surface water protection program. The Act directed the agency as follows: It is the policy of this state and the purpose of this Act to maintain the quality of the water in the state consistent with the public health and enjoyment, the propogation and protection of terrestrial and aquatic life, the operation of existing industries, and the economic development of the state; . . . and to require the use of all reasonable methods to implement this policy." The agency under the "all reasonable methods" clause uses a permit system as its basic regulatory device to control the point discharge of pollutants. Obviously, if you restrict the discharge of pollutants, the Act will require the expenditure of public and private funds for wastewater treatment systems. Therefore, you must know the degree of pollutant discharge restriction in order to avoid wasting resources and whether or not the permits are accomplishing their objective. This was accomplished with descriptive studies of water quality and later with mathematical modeling.

The first modeling endeavors by the Texas Water Quality Board were conceptual models prepared by consultants. During these early endeavors, the reports or users manuals were complicated with technical language. The model limitations were often not explained. This required the users to contact the consultants for assistance. Due to these early problems, many people at the state level failed to accept mathematical models of water quality as useful decision making tools.

Planning Aspects of Public Law 92-500

The Federal Water Pollution Control Act Amendments of 1972 (FWPCAA) established numerous requirements the States would need to satisfy in order to be eligible for construction grant and program grant funds from the Environmental Protection Agency.

The period of 1973-1977 is generally referred to as Phase I of the Act's implementation. In Phase I, the emphasis has been on issuing discharge permits and making construction grants in order to control point sources of pollution which are easily identifiable and correctable. For many areas of the nation, the achievement of this requirement will be all that is necessary for attainment of the 1983 goal.

In Phase II (1978-1983), the emphasis will be on solving the more severe and complex problems produced by point and nonpoint sources of pollution. The identification of the programs necessary in achieving the 1983 goal in complex problem areas is to be accomplished through the preparation of plans required by Section 208 of the Act.

Section 303 of the Act sets forth requirements for each State to establish water quality standards and implementation plans. Under this section each State is required to have a continuing planning process which will result in plans for all navigable waters within the State. These plans are required to contain certain items including the following: 1) total maximum daily load of pollutants for waters which cannot achieve water quality standards using the minimum wastewater treatment levels set forth in the Act, 2) adequate implementation for revised or new water quality standards, and 3) controls over the disposition of all residual waste from any water treatment processing.

Pursuant to Section 303, the EPA issued regulations on State Continuing Planning Process (40 CFR Part 130) and Preparation of Water Quality Management Basin Plans (40 CFR Part 131). These regulations require that revisions to basin plans after July 1, 1975, shall "reconsider current actions with respect to the most recent data or analysis and shall concentrate, if appropriate, on the identification and evaluation of methods and procedures (including land use requirements) to control, to the extent feasible, non-point sources of pollution". The current 40 CFR 130 and 131 guidelines also include the planning requirements of Section 208 of the Act.

For each stream segment with water quality problems caused by nonpoint source discharges, the following minimal information is required: 1) type of problem; 2) identification of waters affected; 3) identification of nonpoint discharges contributing to problem; and 4) alternative procedures and methods (including land use requirements) to feasibly control significant nonpoint source discharges (this evaluation should consider the technical, legal, institutional, economic, and environmental feasibility). The 40 CFR Part 131 regulations further specify that controls over residual wastes be included in basin plans. Residual wastes to be considered include all residual waste from any municipal, industrial or other water or wastewater treatment processing. The regulations also address land and subsurface disposal practices. Basin plans are required to establish a process to control the disposal of pollutants on land or in subsurface excavations wherever such disposal causes or may cause violation of water quality standards or materially affect groundwater quality.

There are two types of areawide planning in which the TWQB is involved - Designated Areawide Planning and Planning in Non-Designated Areas.

> Designated Areawide Planning is the planning required in areas designated by the Governor as having substantial water quality problems as a result of urban-industrial concentrations or other factors. Eight areas have been designated as 208 areas.
>
> Planning in Non-Designated Areas is the planning required in all other areas of the State that are not considered to have substantial water quality problems. These are considered to be State planning areas in which the Texas Water Quality Board is the Planning Agency.

The level of detail of planning for each State planning area will be contingent upon the type and complexity of problems in the planning area, and consequently, the planning tools that are required differ from one area to another.

The purpose of 208 type planning is to: 1) develop methods of achieving or maintaining adequate water quality in the Nation's streams, and 2) insure that construction grant funds spent on construction of domestic sewage treatment plants are spent in a cost effective manner.

In other words, through this planning process should be determined such things as whether or not any particular stream has the ability to meet 1983 stream standards through the application of effluent limitations on dischargers or whether that particular stream is beyond the point of ever meeting existing stream standards for current designated uses. In fact, the most current EPA regulations (40 CFR 130) indicate that a State may establish less restrictive uses than those contained in existing water quality standards by demonstrating one of the following: 1) existing designated use is not attainable because of irretrievable man-induced conditions, 2) existing designated use is not attainable because of natural background, or 3) the application of effluent limitations for existing sources more stringent than those required pursuant to the EPA Effluent Limitation Guideline program in order to attain the existing designated use would result in substantial and widespread adverse economic impact (of course, in order to make these kinds of determinations, both point source and nonpoint source modeling efforts will be required in these determinations).

The nonpoint source pollution program is an integral part of the basin planning and areawide planning programs. The FWPCAA requires a nonpoint source program element in all areawide plans conducted in areas designated pursuant to Section 208(a)(2). In developing the nonpoint source planning element in the Basin Plan, the nonpoint program in the designated 208 areas can be more closely coordinated with the other nondesignated areas. Basin planning regulations require a nonpoint source program element for each water quality segment in which nonpoint source discharges contribute to the water quality problem.

The nonpoint source discharge program will also provide valuable input to, or require input from, other State programs:

1. Water quality standards must reflect achievable goals. At such time as these standards are revised consideration will be given to the impact of nonpoint source discharges on water quality and the feasibility of controlling such discharges.
2. Waste load evaluations should reflect the contribution of nonpoint source discharges to the total load. Detailed information on the origin, magnitude, and frequency of nonpoint source discharges will improve the accuracy and reliability of water quality models.
3. The feasibility of controlling nonpoint source discharges will influence treatment level requirements for point source discharges.
4. In some cases, waste control orders (discharge permits) will be required for nonpoint source discharges.
5. Monitoring programs should be adequate to assess the magnitude and frequency of significant nonpoint source discharges. Either routine monitoring or special surveys may be required to fulfill this requirement.

As indicated earlier, both traditional steady-state point source modeling as well as non-steady state runoff type modeling is required to achieve the integration of a viable point and nonpoint source control program.

The Role of Modeling in Water Quality Management After Public Law 92-500

Each year the Texas Water Quality Board is called upon to develop a statewide water quality management program which can successfully provide guidance in the implementation of the Texas Water Quality Act and the FWPCAA. The aim of this program is to: first, bring about an improvement in water quality in areas where violations of the Texas Water Quality Standards are known to exist and secondly, to preserve the existing quality of the navigable waters of the state where conditions are already acceptable, and further, to implement the necessary requirements for areawide and basin plans in order to insure good water quality in the future.

One of the main efforts toward meeting these objectives lies in preparation of waste load evaluations as required by the FWPCAA Section 303(d)(1)(C). These waste load evaluations as previously mentioned become a part of the Basin plans, as basin planning strategy. They are taken into account during consideration of permit applications as well as determination of new stream standards.

Routinely waste load evaluations will be updated or revised as necessary to accomplish national water quality objectives in conformity with the requirements of the Act and the Continuing Planning Process. For critical segments within each 208 Designated Area, these updates are currently underway.

Texas has twenty-three designated river basins which have been further divided into 297 discrete hydrologic segments. Of these, 230 or 78 percent are considered as "effluent limited" where the minimum treatment required by law will accomplish our stream standards. The remaining 67 segments or 22 percent are considered "water quality limited" where a higher level of treatment is required to meet the desired stream standard. Since the start of implementation of the FWPCAA, 89 waste load evaluation reports have been prepared. Of these, 59 segments were water quality limited while 30 were effluent limited.

A determination of the assimilative capacity of a stream segment requires the quantitative assessment of the effects on the environment of various alternative measures. This is the forte' of mathematical modeling. As such, modeling plays a significant role in the decision making process of several facets of Texas Water Quality Board activities, especially the formulation of waste load evaluations and the issuing of waste discharge permits.

The assimilative capacity of a stream is determined in some cases by complex mathematical models utilizing digital computers; while in other situations, simple engineering calculations are used. This leads us to a categorization, or hierarchy of available steady-state models to be used in the management process.

The first type of model, the type that has the greatest weight in the decision making process, is the model that is completely calibrated and verified for a particular stream segment. This type of model would have been verified during several different flow conditions with predictions closely approximating known conditions.

The second level of model is somewhat simiilar to the first, but lacks verification while being adequately calibrated. This type of model may have been partially verified for only one flow condition.

The third level in the hierarchy of models is that model which has neither been calibrated nor verified, but has been developed with "text-book" or assumed values. This type of model would not have had its predictions matched with actual conditions, nor would it have utilized actual load input conditions but only estimations of what the loads might have been at a given time.

The fourth and lowest level of modeling, although frequently used for the first rough cut at solving dissolved oxygen problems, is the model that does not actually mathematically account for the transport of waste materials, but computes the assimilative capacity of a body of water assuming the body of water is a completely mixed reactor. This type of model is useful for identifying a target load for a stream segment and gives the user an idea of the magnitude of the problem which must be solved.

An example of the first level of modeling would be the Houston Ship Channel model prepared during the Galveston Bay Project. This model was verified numerous times for steady-state conditions. Very few other bodies of water have been modeled to this extent. The second level of modeling is typified by the well-known QUAL-I or QUAL-II type models when flow and loading data is somewhat limited. The third level might be QUAL-I with assumed values for much of the input data. The fourth level is based on the amount of oxygen that can enter through the water surface.

Each level of modeling is useful, for different purposes, and has a place in sound water quality management. For instance, relatively great reliance can be put on the predictive capacity of a level 1 model for analyzing alternative water quality management actions. Treatment levels can be closely evaluated for waste load allocations with only limited additional input required for management decisions, these additional inputs being principally cost of treatment and benefits of maintenance of water quality. For a level 2 modeling situation, less reliance can be placed on model output, and consequently, other factors may take on more weight when considering possible alternatives. These factors include overall water quality considerations as well as cost of control measures. When a 3 or 4 type modeling effort is employed, the management decision is usually of the nature of requiring step wise reductions in waste loading, followed by an evaluation of stream quality response, and then a further control action should the initial step prove unsuccessful.

It should be noted here that the Quality Board does not rely solely on model predictions during the planning process. This would be not only unsound, but also unwarranted. Indeed, all information available should be considered. Consequently, public hearings are conducted by the Texas Water Quality Board after dissemination of engineering reports concerning the modeling and water quality management decisions under consideration for implemention. These hearings work in two ways. That is to say, the Texas Water Quality Board gains additional pertinent information, and at the same time, provides the interested public with a better knowledge of what has gone on during the decision making process.

Problems more complex than determining the total assimilative capacity of a stream segment are: 1) How should the total assimilative capacity be divided among the various waste discharges, and 2) How much allowance for expansion should be provided?

In dividing the assimilative capacity among dischargers we have strived for an equal effort among all dischargers. Some dischargers, however, feel that we have picked on them or that the assimilative capacity has been divided inequitably. In some areas where the majority of pollutant loadings comes from municipal discharges, we have taken a position that the larger plants which account for the majority of the total load should be required to improve their wastewater treatment. An example of this is the Dallas-Fort Worth Area where 4 large wastewater treatment plants account for approximately 90 percent of the total organic load while the remaining 5 small plants account for approximately 10 percent of the loading. The four large plants are required to discharge an effluent with a BOD_5 of not more than 10 mg/l on a monthly average basis while the five small plants may discharge an effluent BOD_5 of 20 mg/l on a monthly average basis.

In areas dominated by industrial discharges, we generally use as a starting point the U.S. Environmental Protection Agency's industrial effluent guidelines. Federal law has required the EPA to define for most industrial categories what are known as: 1) Best Practical Treatment, and 2) Best Available Treatment. These guidelines were developed to impose an equal effort in waste treatment on each type of industry. In the most complex waste load allocation performed by this Agency, the Houston Ship Channel, where 165 wastewater treatment plants and 206 industrial discharges were involved, the assimilative capacity was divided up among the various industries by requiring each to provide treatment such that all discharges are an equal percentage of the differential between best practical and best available treatment. This is illustrated mathematically by the following equation:

$$\text{Allowable Discharge} = \text{BPT} - \frac{X}{100}\ (\text{BPT} - \text{BAT})$$

where:

BPT = best practical treatment

BAT = best available treatment

X = percent reduction required

Over a period of time, the waste loading to any given stream is constantly changing. Therefore, as a waste load allocation is developed, a buffer for growth of existing waste dischargers and the addition of new dischargers to a stream segment is included. This buffer is to insure that as additional loads are imposed upon the stream, the stream is not immediately out of compliance. However, as this buffer is consumed and as the quantity of waste loads approaches the calculated assimilative capacity of the stream, the staff of TWQB must be aware so that further action (either continued monitoring if the water quality is acceptable and not deteriorating or additional waste load allocations) can be taken. Consequently, the TWQB has developed an automatic data processing system to account for the current waste load conditions on a stream segment and to compare existing conditions of loading to the waste load allocation. By using this system, it is possible to quickly determine potential problem areas and to establish priorities for analysis of stream segments utilizing limited engineering resources.

The modeling work previously discussed covers Phase I of the FWPCAA. The Texas Water Quality Board is presently in the development of methodology stage of modeling for the 208 areawide planning program. The types of models that will be used are discussed briefly under modeling inventory.

Modeling Inventory

Over the last four years, the Texas Water Quality Board has acquired a number of computer models for use in the various water quality management tasks given to us. The models vary in complexity from simple one-dimensional steady-state river models to two-dimensional and time variable estuarine models.

Our general purpose models include: 1) the QUAL models - developed by the Texas Water Development Board and modified by Water Resources Engineers, Inc., 2) the AUTO-QUAL models - developed by the Environmental Protection Agency, and 3) the ESTPOL models - developed by Texas A&M University. The primary use of these models is in the waste load evaluation work performed by the Texas Water Quality Board. These are basically steady-state applications.

In time variable applications, the TWQB is now applying or evaluating 1) the AUTO-QUAL model; 2) the STORM model - developed by Water Resources Engineers, Inc.; 3) the STORM WATER MANAGEMENT model - developed by Metcalf & Eddy, Inc., the University of Florida, and Water Resources Engineers, Inc.; and 4) RECEIV II - developed by Ratheon for the EPA. One or more of these models will be used in the upcoming 208 program dealing with nonpoint waste loadings.

The TWQB has acquired two general purpose lake models. These are 1) EPARES, and 2) RIVER-RESERVOIR, both developed by Water Resources Engineers, Inc. We have not yet had the opportunity to use either of these models, but we have tried to become familiar with their basic features.

At times the TWQB has turned to basin specific models to solve particular water quality management problems. The largest example of this type of work has been the Galveston Bay Project. In this project, a two-dimensional model of Galveston Bay was developed along with a one-dimensional steady-state model of the Houston Ship Channel. The development of these models was accomplished by Tracor and Hydroscience, Inc. The ship channel model was used in the waste load evaluation of that segment. Hydroscience, Inc. has also developed a basin specific model for the Trinity River and they are presently under contract to develop an eutrophication model of Lake Livingston, a 82,600 acre lake northeast of Houston. The TWQB continues to look for new models and for new applications of existing models.

A DYNAMIC WATER QUALITY SIMULATION MODEL FOR THE THAMES RIVER

D. G. Weatherbe
Water Resources Branch
Ontario Ministry of the Environment
Toronto, Ontario

Summary

The Thames River basin is experiencing problems of water quality and flooding, heightened by intensive agricultural use and an expanding urban population. A study was initiated to provide solutions to these problems as well as problems of erosion, unsatisfied recreational demand, and conflicts in reservoir use. In order to provide a suitable tool for the analysis and projection of the water quality problem, a dynamic water quality simulation model was developed and applied to the major growth center, the City of London. This paper describes the major objectives of the water quality modelling, the model structure and processes, as well as model input and output summaries. The application of the model to evaluate various water quality management options is described.

Need for a Study

The river experiences water quality impairment problems caused by excessive inputs of nutrients, oxygen demanding materials, bacteria and suspended solids from urban and rural sources. The largest city in the basin, the City of London, is expected to grow from a population of 220,000 in 1971, to 500,000 in 2001, with a proportional increase in sewage discharges to the river. Options for controlling present and future problems for the City of London consisted of increased levels of sewage treatment, sewage diversion directly to Lake Erie by pipeline, low flow augmentation from proposed reservoirs and urban growth restrictions. This part of the study was initiated primarily to evaluate these water quality options.

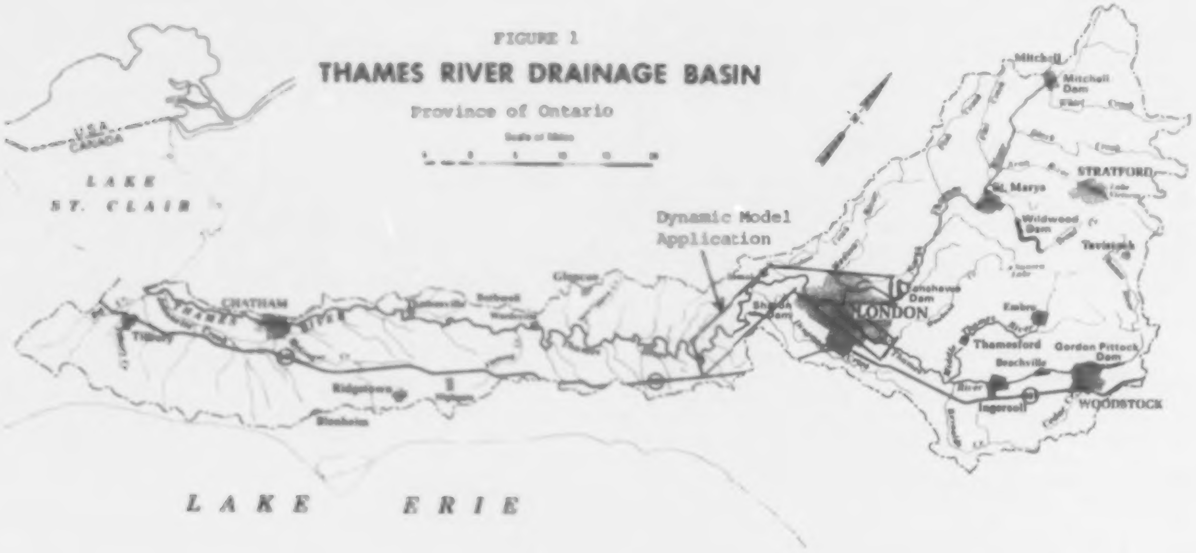


FIGURE 1
THAMES RIVER DRAINAGE BASIN
Province of Ontario

Thames River Study

Basin Description

The Thames River in southwestern Ontario (Fig. 1), drains 2,250 square miles of mainly agricultural land with a total 1971 population of 415,000, 334,000 in urban areas and 81,000 in rural. Major surface water uses include those for sewage disposal, recreation and fish and wildlife habitats. Municipal water supplies are either of ground water origin or are imported from the Great Lakes by pipeline. Three multiple use reservoirs in the basin, with a maximum combined storage volume of 72,500 acre-feet, are used for flood control, low flow augmentation and recreation.

Study Objectives

General - The overall objective of the study was "to develop guidelines for the management of the basin's water resources to ensure that adequate quantities of water of satisfactory quality are available for the recognized uses at the lowest possible cost, and that erosion and flood protection are provided consistent with appropriate benefit-cost criteria"[1].

Water Quality Objective - The general water quality objective defined during the study was to maintain existing water quality where it is satisfactory for fish and aquatic life and recreation, and to improve quality to that level in those areas where it is presently degraded.

Appropriate dissolved oxygen criteria to achieve this objective were identified for major sections of the river, based on published Ontario guidelines[2]. These criteria were redefined in statistical terms to allow comparison with model output summaries. For example, Criteria C, which represents an acceptable quality of water with some stress, to be applied for warm water fish species in non-spawning periods, is stated as follows: "the dissolved oxygen concentration should be above 5 mg/l 95 percent of the time in a given month. Concentrations may range between 5 mg/l and 4 mg/l for periods up to four hours in length within any 24 hour period, provided that water quality is favourable in all other respects".

Dynamic Water Quality Simulation Model

Model Description

The dissolved oxygen model used in the Thames River Study takes account of the effects of carbonaceous and nitrogenous oxygen demand, atmospheric aeration, aeration at weirs, respiration in bottom sludges, photosynthetic oxygen production, and respiration of aquatic plants and algae. Model parameters are adjusted to account for the effect of changes in temperature and channel flow.

The model expressed as a differential equation, in terms of the oxygen deficit D, is given below as a function of time, t, and distance, x. The oxygen deficit D is the difference between the oxygen saturation concentration and the actual concentration.

$$\frac{\partial D}{\partial t} + \frac{V\partial D}{\partial x} = -KaD+KdL(x)+KnN(x)+S - P(t)+R$$

where:

D =oxygen deficit, mg/l
V =velocity of stream, ft/sec
t =time, days
x =distance, ft
Ka =aeration coefficient, day^{-1} (O'Connor and Dobbins, 1958)[3]
Kd =deoxygenation coefficient, day^{-1}
L(x) =carbonaceous oxygen demand as a function of x, given by L(x)=Lo $e^{-Kn(x/V)}$
Lo =initial concentration of carbonaceous oxygen demand, mg/l
Kr =oxygen demand removal coefficient, day^{-1}
N(x) =nitrogenous oxygen demand as a function of x, given by N(x)=No $e^{-Kn(x/V)}$
No =Initial nitrogenous oxygen demand, mg/l
Kn =nitrogenous oxidation coefficient, day^{-1}
S =benthic bacterial respiration, mg/l/day
P(t) =photosynthetic oxygen source as a function of time, of the form $P(t)=Pm \sin |(\pi/p)(t-ts)|$ for daylight hours. A step function approximation F(t), of the function P(t) is used which assumes a constant rate of photosynthesis over a time step, h (two hours)
Pm =maximum rate of photosynthetic production, mg/l/day
p =period of sunlight, days (fraction)
ts =time of sunrise, days (fraction)
R =algal respiration, mg/l/day

This formulation and solution are as expressed by O'Connor and DiToro (1970)[4] except for the step function, F(t).

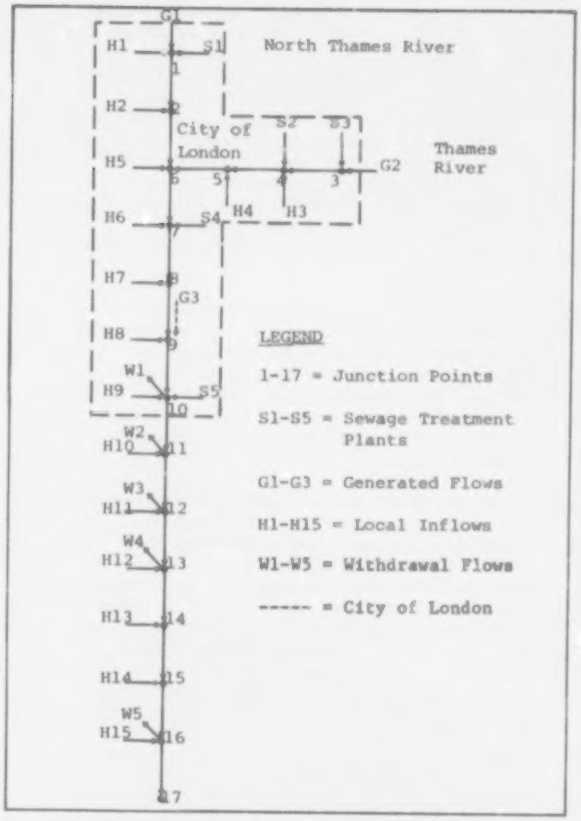


Figure 2: Thames River water quality simulation model - geometry of river system.

River System Geometry

The dissolved oxygen levels throughout a river are described by treating the river as a collection of reaches with constant conditions in each reach, calculating the effect of all input and withdrawals at the head of the reach and using the model formulation to calculate the concentrations of dissolved oxygen and waste constituents at the end of the reach. Weir aeration is assumed to take place at the head of the reach[5]. Figure 2 shows the geometry of the river system modelled, indicating the reach junctions, sewage treatment plant inputs, local inflows (tributaries), withdrawal flows and upstream flows.

Input Variations

The dynamic water quality simulation model was developed to take account of the variations of natural and man-made conditions that affect water quality, to provide increased information about the possible effects of water management planning alternatives in the river basin. The inputs to the system vary with time to reproduce the variations in conditions that occur in the real system. Causes of variation in water quality accounted for in the dynamic simulation model, include:

i Streamflow from the upstream main channel and from tributaries. Daily streamflows were generated for the upstream gauge locations, based on the historical record. The method generates extensive traces of streamflow data from available historical records using stochastic techniques and thus allows the water quality simulation model to be run for as long a period as required (Singer, 1974)[6]. Channel flow velocities, aeration rates, respiration rates and photosynthetic rates are affected by changes in streamflow.

ii Water quality from upstream and from tributaries. Probability distributions based on observed water quality are used in the model to reproduce daily variations in dissolved oxygen (DO), carbonaceous (CARBOD) and nitrogenous oxygen demand (NOD). Diurnal variations of dissolved oxygen are also included.

iii Waste treatment plant loads. Observed daily mean effluent flows are reproduced by mathematically describing seasonal and within-week trends and adding a random component. Within-day variations in treatment plant flows are also included. Daily mean water quality parameter concentrations (DO, NOD, CARBOD) are randomly chosen from probability distributions based on observed data. Table 1 describes the probability distributions for the water quality of the main channel flows and sewage treatment plants.

iv Sunlight energy. A probability distribution of sunlight energy for each month is used to calculate variations in the average photosynthetic rates of plants and algae for each reach, and each day.

v Temperature. Mean daily water temperatures are calculated in the model according to observed trends. Oxygen saturation concentrations, aeration rates and respiration rates depend on temperature.

Model Application

Model Runs

Computer simulation runs were undertaken to evaluate various cases defined by input conditions. Each run consisted of the simulation of dissolved oxygen, carbonaceous and nitrogenous oxygen demand at each reach node, every two hours, for thirty years, for each month simulated. Typically, the critical months of May, June, July and August were simulated.

Input conditions for streamflow, sewage treatment quality, sewage flow, and sewage outfall location were altered to define various management possibilities as outlined below:

Streamflow - Cases modelled consisted of unregulated flows generated from historic records, regulated flows from the operation of three existing reservoirs and regulated flows from the addition of two proposed reservoirs.

Sewage Treatment Quality - Cases modelled consisted of existing quality as described in Table 1, based on 1972 data, improved quality consisting of nitrified secondary effluent approximated by the quality of Greenway STP, shown in Table 1 and zero pollutants defined by negligible concentration of pollutants and high effluent dissolved oxygen.

Sewage Flow - Cases modelled were existing (1972) flow rate with a total of 27.6 MIGD (51.2 cfs) on the average and 1991 project sewage flow rate of 49.5 MIGD (92 cfs).

Sewage Outfall Location - Cases modelled were existing (1972) with 1991 flows distributed to existing STP's on a proportional basis, a new plant downstream accepting all flow increases and complete sewage diversion to Lake Erie.

Model Output - For each month and each reach, the model printout tables consisting of the number of violations of dissolved oxygen criteria, the distribution of and average duration of violations,

TABLE 1: Thames River Simulation, Water Quality Inputs, Description of Probability Distributions and Mean Sewage Flows

Input Location	Carbonaceous O.D.[a] 10%[c] (mg/l)	Median (mg/l)	90% (mg/l)	Nitrogenous O.D.[b] 10% (mg/l)	Median (mg/l)	90% (mg/l)	Daily Mean Flow[d] 1972 (cfs)
Adelaide STP	13.4	30.0	68.0	59.4	98.0	125.0	5.1
Pottersburg STP	12.0	35.0	109.0	11.2	45.0	114.0	6.6
Vauxhall STP	15.8	40.0	98.0	20.3	64.0	98.0	6.3
Greenway STP	8.0	20.0	54.0	4.7	7.0	23.0	32.0
Oxford STP	10.0	20.0	44.0	60.7	123.0	180.0	1.4
North Thames R.	1.2	1.8	5.2	2.4	3.2	6.6	---
Thames R. (S. Branch)	1.0	1.6	3.3	2.6	3.2	4.9	---

Notes:

a Carbonaceous oxygen demand, (CARBOD) estimated by multiplying BOD_5 data by the $CARBOD/BOD_5$ ratio determined through laboratory analysis. Ratio of 2 for the STP's and 1 for the stream inputs were used.

b Nitrogenous oxygen demand, (NOD) determined by multiplying Kjeldahl nitrogen data by 4.57, the ratio of NOD to unoxidized nitrogen, determined by stoichiometric balance.

c 10 percent of observations did not exceed value.

d Based on the period from May to October 1972

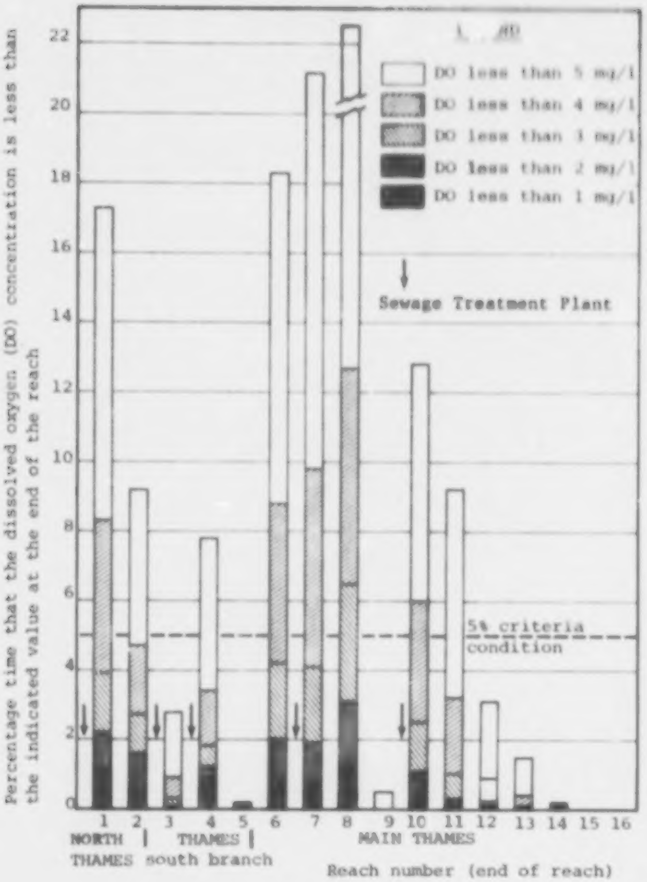


Figure 3: Thames River water quality simulation model - dissolved oxygen output summary for the month of July based on inputs for existing conditions (1972).

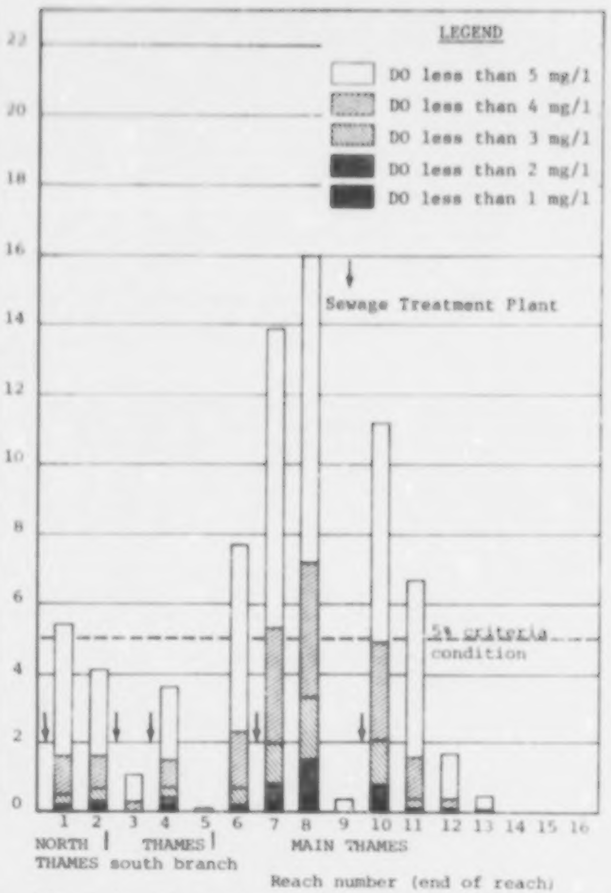


Figure 4: Thames River water quality simulation model - dissolved oxygen output summary for the month of July, based on input conditions of improved quality effluent, existing sewage flow, existing dam operation, existing outfall location.

and the total time in violation. Optional output consists of cross tabulations of output parameters (dissolved oxygen, carbonaceous and nitrogenous oxygen demand) with streamflow for each reach, and a plot of output parameters.

Existing Conditions - The output table showing the percent time in violation is shown graphically in Figure 3 for the existing conditions, defined by the model input combination of regulated flow, existing sewage quality, existing sewage flow and existing outfall locations. The criteria condition that allows occurrences of dissolved oxygen less than 5 mg/l for 5 percent of the time is also shown. From this, it can be seen that significant criteria violations occur in eight of the sixteen reaches.

Model Verification - The model is constructed with calibrated parameters based on actual surveys and actual data are used in the input variations. Consequently, results are thought to represent the real conditions. Intensive survey data, and long term monitoring data confirm that a dissolved oxygen problem exists; however, continuous data comparable to model output are presently not available for verification. The model provides the "best" estimate of water quality, but the absolute values predicted cannot be verified. Consequently, the model is most useful for comparing the relative effectiveness of optional control measures.

Conclusions Derived from Model Applications

Existing Conditions - Dissolved oxygen conditions presently represent an unacceptable quality. Urban expansion without improvement should not be allowed.

Nitrification - Improvement of sewage quality by nitrification of effluents significantly improves water quality in the river. Figure 4 shows the predicted water quality resulting from nitrification of effluents. The model predicts an insignificant negative effect from increased sewage flows when only nitrified effluents are discharged.

Zero Pollutants - Treatment to a zero pollutant level further improves water quality, however, violations are still predicted by the model. This is due to the combined effects of upstream quality and algal and sludge respiration.

Flow Augmentation - The addition of upstream reservoirs operated to provide flow augmentation would significantly improve water quality.

Outfalls - The location of sewage outfalls within the city causes no significant difference in water quality. Diversion of sewage to Lake Erie would improve quality, but not to the level provided by treatment to a "zero pollutant" level. This is because diversion of sewage reduces both the waste load and the flow to the river.

Verification - Dissolved oxygen data of a continuous nature are required for proper verification of the model (a continuous monitor was installed in 1974).

Urban Runoff - The model parameters and input variations include the indirect effects of urban runoff which were present in the stream during intensive surveys; however, the urban runoff effect is inseparable from other effects. Consequently, studies are being undertaken to determine the significance of this source.

Eutrophication - The effects of nutrient controls on dissolved oxygen could not be estimated, since no quantification was available for the nutrient plant growth - dissolved oxygen relationship. Studies are being undertaken to investigate this phenomena.

Waste Loading Guidelines

Conclusions derived from model runs were used in the statement of allowable waste discharge rates for each reservoir construction alternative. These statements, called waste loading guidelines, are based on loading rates which produce marginally acceptable water quality. The loading rate, which produced the model output shown in Figure 4 was considered marginally acceptable, in spite of the predicted criteria violations, because of the lack of model verifications and since treatment to the zero pollutant level or diversion still produced criteria violations. An arbitrary limit on the dilution ratio acceptable at low flow was also incorporated in the identification of allowable waste discharge rates as follows: tertiary treatment (to stream quality - approximately 15 mg/l total oxygen demand) should be initiated when the dilution ratio of stream flow to sewage reaches 1.5:1, and increases in discharge should stop when the dilution ratio reaches 1:1.

"System Options", which were combinations of a waste disposal option and a reservoir construction option were defined on the basis of the above analysis. Water quality benefits were assumed to be constant for all options. The present value of costs for each option was estimated at various interest rates, including the negative costs (i.e. benefits) from flood control. A least cost ordering of the options then provided input to a subsequent analysis of unquantified costs and benefits for various options.

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DISPERSION MODEL FOR AN INSTANTANEOUS SOURCE OF POLLUTION
IN NATURAL STREAMS AND ITS APPLICABILITY TO THE
BIG BLUE RIVER (NEBRASKA)

Mahendra K. Bansal, Ph.D., P.E.
Nebraska Natural Resources Commission, Lincoln, Nebraska

Summary

Dispersion behavior in natural streams depends upon dispersion rates, channel configuration, turbulent flow characteristics, and biochemical changes taking place in the stream environment. This is true for an instantaneous source of pollution for all times. This also holds good for a continuous source of pollution during transition periods when mixing is not complete in the reach. Therefore, the prediction of turbulent dispersion coefficients is important in the determination of water quality constituent concentration in natural streams. However, the longitudinal dispersion rates predicted by the QUAL model are low, which results in higher concentration peaks of short durations. In steady-state conditions, for a continuous plane source of pollution, the dispersion behavior in natural streams does not depend upon the dispersion rates. Under these conditions, an exact solution of the dispersion equation is available, and as such a finite-difference approximation technique should not be used. One- and three-dimensional mathematical models of dispersion are presented in this study. The turbulent dispersion coefficients calculated were tested for the Big Blue River in Nebraska. The dispersion model developed is not dependent on channel size or regional location of the stream.

Introduction

A pollutant, whether agricultural or domestic, municipal or industrial, hot or cold, when discharged into a stream, will mix and disperse according to turbulent flow characteristics of the stream. Presently, significant advances have been made in the understanding of the basic mechanism of dispersion, but the problem of predicting the time-concentration distribution of a water quality constituent still remains to be settled. There are some dispersion models available, but their applicability is often limited.

The U. S. Environmental Protection Agency, in its effort to deal with the stream pollution under Section 303 of the Federal Water Pollution Control Act Amendments of 1972, adopted the QUAL-I and QUAL-II models to help in formulation of the water quality management plans for various river basins in Nebraska and other states. The water quality model, QUAL-I[1,2], was designed to simulate the dynamic behavior of conservative minerals, water temperature, carbonaceous BOD, and dissolved oxygen levels in various segments of natural streams. The QUAL-II[3] model, which is a modified version of the QUAL-I model, additionally simulates benthal oxygen demand, nitrogenous BOD, phosphorous, coliforms, chlorophyll-A, and radioactive constituents in natural streams. The simulation of the dispersion component are identical in the QUAL-I and QUAL-II models.

The Nebraska Natural Resources Commission, on request from the State Department of Environmental Control, tested the suitability of QUAL-I and QUAL-II models in simulating the dynamic behavior of conservative minerals in the Big Blue River in Nebraska. The time-of-travel data[4], gathered by the U. S. Geological Survey on the Big Blue River during August 1973 and May 1974, were analyzed to respond to the turbulent dispersion dynamism in natural streams.

Mathematical Model of Dispersion

The concentration distribution of a water quality constituent in turbulent streams is governed by the law of conservation of mass. The diffusive mass-transport equation for a conservative pollutant, where there are no bio-chemical changes taking place in the stream environment, assuming longitudinal flow and no other sources and sinks in the reach, is:

$$A\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(A\bar{u}c) = \frac{\partial}{\partial x}(AD_x\frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(AD_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(AD_z\frac{\partial c}{\partial z}) \;. \;. \; (1)$$

where c = local mean concentration; x, y, z = spatial coordinates in longitudinal, lateral, and vertical directions, respectively, measured from the center of stream surface as datum; $\bar{u}$ = mean flow velocity in longitudinal direction; D_x, D_y, D_z = turbulent diffusion coefficients in x, y, z directions, respectively; and t = time elapsed since injection of the pollutant or dye in a natural stream. Equation 1 is based on the Fick's law of diffusion where the transport associated with the turbulent fluctuations is proportional to the concentration gradient. For one-dimensional flow, the diffusive mass-transport equation reduces to:

$$A\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(A\ V\ c) = \frac{\partial}{\partial x}(A\ D_L\ \frac{\partial c}{\partial x}) \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; (2)$$

where D_L = longitudinal dispersion coefficient; and V = average velocity of flow in the reach. Equations 1 and 2, assuming dispersion coefficients are constant in a reach, correspond to:

$$D_L = D_x + (D_y\frac{\partial^2 c}{\partial y^2} + D_z\frac{\partial^2 c}{\partial z^2}) / \frac{\partial^2 c}{\partial x^2} \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; (3)$$

For sampling stations far downstream of the injection site, where mixing in the lateral and vertical directions is almost completed, it can be assumed that $D_L = D_x$, because:

$$\frac{\partial^2 c}{\partial x^2} >> \frac{\partial^2 c}{\partial y^2}, \frac{\partial^2 c}{\partial y^2} .$$

Otherwise, D_L would remain a function of D_x, D_y, D_z, $\partial^2 c/\partial x^2$, $\partial^2 c/\partial y^2$, $\partial^2 c/\partial z^2$, and non-linearity of flow. In this study, D_L is taken to be a function of D_x, and $\bar{u}/V$.

Instantaneous Source

Let M be the amount of conservative constituent injected as a plane source at any point of the stream. The initial and boundary conditions are:

$c(x,0) = 0$ for all x,

$\int_{-\infty}^{\infty} A(x)\ c(x,t)dx = M -$ constituent losses in the reach for all t,

$c(\infty,t) = 0$ for all t,

$\frac{\partial c}{\partial x} \rightarrow 0$, as $t \rightarrow \infty$.

The solution of Eq. 3 that satisfies the above conditions, is well known and is given by,

$$c(x,t) = \frac{M}{A\sqrt{4\pi D_L t}} \exp\left[-\frac{(x-Vt)^2}{4D_L t}\right] \text{ - losses in the reach.} \quad \ldots\ldots (4)$$

The one-dimensional mathematical model of dispersion, which is also a solution of Eq. 3, adopted in this study is:

$$c = \frac{M}{A\sqrt{4\pi D_L t}} \exp\left[-\frac{(x-Vt)^2}{4D_L t} - \frac{k_0 Vt}{L}\right] \quad \ldots\ldots\ldots (5)$$

where k_0 is a loss factor and L is some characteristic length. In this study, k_0 is kept unity, and L is taken equal to x. If the value of D_L is known for a reach, the concentration distribution can be computed from Eq. 5.

The three-dimensional model of dispersion, which is a solution of Eq. 1, adopted in this study is:

$$c(x,y,z,t) = \frac{M}{A\sqrt{4\pi D_L t}} \exp\left[\frac{-(x-Vt)^2}{4D_L t}\right] \frac{2B}{\sqrt{4\pi D_y t}} \exp\left[\frac{-y^2}{4D_y t}\right]$$

$$\frac{2H}{\sqrt{4\pi D_z t}} \exp\left[\frac{-z^2}{4D_z t}\right] \quad \ldots\ldots\ldots\ldots (6)$$

To use Eq. 6, three of the four unknowns c, D_L, D_y, and D_z must be known. The value of D_L is first determined from the one-dimensional model of dispersion, and D_y and D_z are considered inter-related. Based on past work, the empirical relationship is taken as,

$$D_y = \left(\frac{\bar{u}}{V}\right)^2 \left(\frac{B}{H}\right)^2 D_z \quad \ldots\ldots\ldots\ldots\ldots\ldots (7)$$

where $\bar{u} = \frac{Q}{A}$, $V = \frac{x}{t_p}$, $H = \frac{A}{B}$; Q, A, B are discharge, cross-section area, and top width of flow; x is the reach length; and t_p is the time to peak arrival of the constituent concentration at a sampling station. The value of D_z which gives the best fit between the computed and measured time-concentration curves, is taken to be the approximate value of D_z for that stream reach.

The empirical equations used in the evaluation of turbulent dispersion coefficients, D_L, D_y, D_z, in the longitudinal, lateral, and vertical directions, based on past work [5,6,7,8] are:

$$\log\left(K \frac{\bar{u}}{V} \frac{D_L}{VH}\right) = 6.45 - 0.762 \log\left(\frac{\rho\ V\ H}{\mu}\right) \quad \ldots\ldots\ldots (8)$$

$$\log\left(K \frac{\bar{u}}{V} \frac{D_z}{\nu}\right) = -8.1 + 1.558 \log\left(\frac{\rho\ V\ H}{\mu}\right) \quad \ldots\ldots\ldots (9)$$

where ρ, μ, and ν are the density, coefficient of viscosity, and kinematic viscosity of flow at stream water temperature; and K is a regional dispersion factor assumed to be unity for the Big Blue River.

Equations 7, 8, and 9 reveal that the dimensionless dispersion parameters are a function of the Reynolds number of flow, and channel configuration of the stream. Knowing the dispersion coefficients, the concentration distribution for an instantaneous source of pollution can be computed at any point of the stream.

Continuous Plane Source

Let m units per unit area of a conservative constituent be dumped at the origin for times t>0 in a stream moving with a uniform velocity $\bar{u}$ in x-direction. The concentration at any point (x,t) due to the constituent m dt' injected during a time element dt' at time t' is:

$$\Delta c = \frac{m\ dt'}{\sqrt{4\pi D_L (t-t')}} \exp\left\{\frac{-\left[x-\bar{u}(t-t')\right]^2}{4D_L(t-t')}\right\}$$

The resulting concentration at time t due to the water quality constituent dumped continuously at origin from time 0 to t, is given by,

$$c = \frac{m}{\sqrt{4\pi D_L}} \int_0^t \exp\left\{\frac{-\left[x-\bar{u}(t-t')\right]^2}{4D_L(t-t')}\right\} \frac{dt'}{(t-t')^{1/2}}, \text{ or}$$

$$c = \frac{mx}{\sqrt{4\pi D_L}} \exp\left(\frac{\bar{u}x}{2D_L}\right) \int_{x/2\sqrt{D_L t}}^{\infty} \exp\left\{-\eta^2 - \frac{\bar{u}^2 x^2}{16 D_L^2 \eta^2}\right\} \frac{d\eta}{\eta^2}$$

$$\text{where } \eta = x/2\sqrt{D_L(t-t')} \quad \ldots\ldots\ldots\ldots\ldots\ldots (10)$$

The exact solution of Eq. 10 is not available, but it can be approximated as,

$$c = \frac{m}{\bar{u}} \operatorname{erfc}\left(\frac{x\ p}{2\sqrt{D_L t}}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots (11)$$

where p is an undefined constant, and erfc is a complementary error function. The value of x must not exceed the characteristic length L after which the mixing in lateral and vertical directions is almost completed. The length L can be taken a multiple of $16D_L/V$. For steady-state conditions, when $t \rightarrow \infty$,

$$c = \frac{m}{\bar{u}} \quad \text{for all } x \quad \ldots\ldots\ldots\ldots\ldots\ldots (12)$$

If M units are the total amount of the constituent concentration dumped in the stream per unit time, then,

$c = \frac{M}{A\bar{u}}$, or c Q = constant, therefore,

$$c\ Q = c_1\ Q_1 + c_2\ Q_2 \quad \ldots\ldots\ldots\ldots\ldots\ldots (13)$$

where c_1, Q_1 = incoming constituent concentration and discharge in the stream; c_2, Q_2 = effluent concentration and flow discharged into the stream; and c, Q = resulting outgoing constituent concentration and discharge downstream of the injection site under steady-state conditions.

Dispersion Component in the QUAL-Model

The diffusive mass-transport equation used in the QUAL-I and QUAL-II models is the same as Eq. 2. A finite-difference method is used for its solution. To avoid instability of solution, an implicit technique of backward-difference approximation is used to solve Eq. 3. The linear equation adopted at time step n + 1 when its spatial distribution for all distance steps i at time step n are known, is:

$$c_i^{n+1} + W_i\ c_{i+1}^{n+1} = G_i^n \quad \ldots\ldots\ldots\ldots\ldots\ldots (14)$$

$$\text{where } W_i = \frac{d_i}{b_i - a_i W_{i-1}}, \quad G_i = \frac{Z_i - a_i G_{i-1}}{b_i - a_i W_{i-1}}$$

$$\text{and} \quad a_i = \frac{\Delta t}{\Delta x^2} D_{L_{i-1}} - Q_{i-1} \frac{\Delta t}{U_i}$$

$$b_i = 1 + \frac{\Delta t}{\Delta x^2} \left(D_{L_{i-1}} + D_{L_i}\right)$$

$$d_i = -\frac{\Delta t}{\Delta x^2} D_{L_i}$$

$$Z_i = c_i^n + \frac{\Delta t}{U_i} \Delta Q_{x_i} \Delta c_{x_i}$$

$$U_i = \frac{1}{2}(A_i + A_{i-1})$$

For a head reach, $W_1 = \frac{d_1}{b_1}$, $G_1 = \frac{Z_1}{b_1}$, and

$$Z_1 = c_1^n + \frac{\Delta Qx_1 \ \Delta Cx_1 \ \Delta t}{U_1}$$

In Eq. 14, c_{i+1}^{n+1} is unknown, therefore, the solution starts backward from the last reach, given by,

$$c_\ell^{n+1} = G_\ell \quad \ldots\ldots\ldots\ldots \quad (15)$$

where $G_\ell = \frac{Z_\ell}{b_\ell}$, and $Z_\ell = c_\ell^n + \frac{\Delta Qx_\ell \ \Delta c_{x_\ell} \ \Delta t}{U_\ell}$

This is possible when $W_\ell = 0$. The assumption of W_ℓ in the last reach to be zero for all time increments is questionable. During initial periods, when mixing is not complete, W_ℓ should not be zero.

A perusal of numerical values of a, b, d, and z would reveal that d is approximately zero for all times, and the resulting concentration can be approximated as,

$$c_i^{n+1} = G_i \text{ for all times} \quad \ldots\ldots\ldots\ldots \quad (16)$$

It is not true for the last reach only as it has been adopted in the QUAL model given by Eq. 15.

It is to be further noted that the QUAL-I and QUAL-II models are designed for a continuous source of pollution. This is evident from the values of Z_i which are computed cumulatively for constituent increaments, Δc_{xi}, injected at origin at time intervals of Δt integrated over 0 to t. However, under steady state conditions, an exact solution is available for a linear uniform flow, given by Eq. 13. In this case, the resulting concentration is not dependent on the dispersion coefficient. Equation 13 is important because steady-state solutions are often required to be studied in evaluation of the water quality management plans.

In the case of a continuous source of pollution, the finite-difference approximate solution is therefore valid only for the transition period during which the mixing is not completed. It should also hold good for an instantaneous source of pollution, where the concentration distribution is dependent on the dispersion rates for all times.

The QUAL model uses the Elder's equation[9] to evaluate the longitudinal dispersion coefficient, described by,

$$D_L = 5.93 \ U_* \ D$$

where U_* is the bed shear velocity, given by $\sqrt{gDS_e}$, and S_e is the energy slope calculated from the Manning's equation. The resulting dispersion equation is expressed as,

$$D_L = 22.6 \ N \ \bar{u} \ D^{0.833} \quad \ldots\ldots\ldots\ldots \quad (17)$$

where N is the Manning's coefficient for the reach.

The mean velocity and depth of flow are calculated from the relationships,

$\bar{u} = \alpha Q^\beta$, and $D = \gamma Q^\delta$

where α, β, γ, δ are constants of proportionality predetermined from the velocity- and stage-discharge rating curves.

The values of longitudinal dispersion coefficients calculated from Eq. 17 and Eq. 8 differ considerably. It is later found that Eq. 17 cannot be used for all the hydraulic flow conditions in natural streams.

Dispersion Simulation in the Big Blue River

A summary of the time-of-travel data and discharge measurements collected by the U. S. Geological Survey between the Seward and Barneston stations on the Big Blue River during August 1973 is given in Table 1. A fluorescent dye, Rhodamine WT, 20 percent solution in acetic acid, was injected at three locations along the river and the fluorescence was monitored at regular intervals for about ten days at fifteen sampling stations, as shown in Fig. 1. It is well known that a natural stream profile is not uniform. Its configuration changes from section to section. There are some dead pockets present in a stream reach, where the dye is detained temporarily and is released at later times. In some cases, the measured concentration curve has two or more peaks. To make the hydraulic data as consistent as possible, the observed top-width and area of cross section of flow are plotted against the measured discharge for each gaging station. Such a plot for the Big Blue River at Crete is shown in Fig. 2, which indicates that the cross-section area is not zero for a zero discharge, and the effective cross section is then determined.

To verify the dispersion model for the Big Blue River, the time-concentration distribution curves were computed from the longitudinal dispersion rates adopted in the QUAL model (Eq. 17) and also from the one- and three-dimensional models of dispersion, Eqs. 5 and 6. They are shown plotted against the site measurements in Figs. 3 and 4, respectively, for the sampling site near Seward. The dispersion coefficients evaluated from Eqs. 7, 8, 9, and 17 are also given in Table 1. It is evident from Fig. 3 and Table 1 that the longitudinal dispersion coefficients computed in the QUAL model are much less than those required to simulate the observed time-concentration distribution. The concentration distribution resulting from the QUAL model, therefore, consists of higher peaks spanning for short durations only. The adoptability of the Elder's equation in simulation of the dispersion component in the QUAL model, therefore, needs further investigations.

In order to verify the applicability of the longitudinal dispersion coefficient predicted from Eq. 8, a test was made to check the response of peak concentration at different locations along the stream. Variations in the computed peak concentrations and the site measurements are shown in Fig. 5 for the stream reach between the Seward and Crete stations on the Big Blue River. Figure 5 indicates that the one-dimensional model of dispersion, Eq. 5, behaved satisfactorily. And the values of longitudinal dispersion coefficients predicted from Eq. 8 agree well with the turbulent dispersion characteristics of the stream.

TABLE 1
TIME-OF-TRAVEL MEASUREMENTS
BIG BLUE RIVER (NEBRASKA)
August 21-30, 1973

Sl. No.	Distance Traversed (miles)	Flow (cfs)	X-section Area (ft^2)	Top Width (ft)	Water Temp. (^oC)	Time to Peak (hrs)	QUAL model Disp. Coeff. D_L (ft^2/sec)	Estimated Dispersion Coefficients (ft^2/sec)		
								D_L	D_Y	D_Z
Dye Dumped at Highway 34 at Seward (amount 6 lb)										
1	1.20	25.50	24.20	36.00	25	3.80	0.92	90.84	0.0368	0.000013
2	5.36	25.00	59.00	38.00	25	28.60	0.91	28.60	0.0031	0.000037
3	20.46	25.00	36.10	32.00	24	91.00	0.91	52.95	0.0103	0.000027
4	25.26	25.00	40.00	36.00	24	197.20	0.91	36.32	0.0279	0.000032
5	31.06	25.00	22.00	24.00	24	232.90	0.91	74.99	0.1046	0.000032
Dye Dumped at Site Below Dam Southeast of Milford (amount 20 lb)										
6	5.80	32.30	27.10	26.00	28	17.00	0.65	123.66	0.0210	0.000027
7	19.76	132.40	103.00	85.00	28	37.00	1.69	171.99	0.1122	0.000029
8	49.00	152.00	85.00	50.00	26	87.00	1.87	293.33	0.0973	0.000057
9	54.15	156.00	100.00	82.00	26	94.10	1.90	227.53	0.1785	0.000031
Dye Dumped at Damsite at DeWitt (amount 35 lb)										
10	5.15	194.00	161.00	110.00	28	6.30	2.21	200.31	0.0586	0.000031
11	23.07	210.00	96.40	79.00	28	32.50	2.23	380.74	0.3572	0.000034
12	29.25	200.00	112.00	110.00	28	45.00	1.78	271.15	0.4411	0.000024
13	32.70	192.00	112.00	127.00	28	67.00	1.73	218.86	0.9610	0.000022
14	38.50	295.00	190.00	126.00	28	90.50	2.27	210.29	0.6905	0.000049
15	48.00	300.00	148.00	86.00	28	161.20	2.29	269.21	1.5992	0.000081

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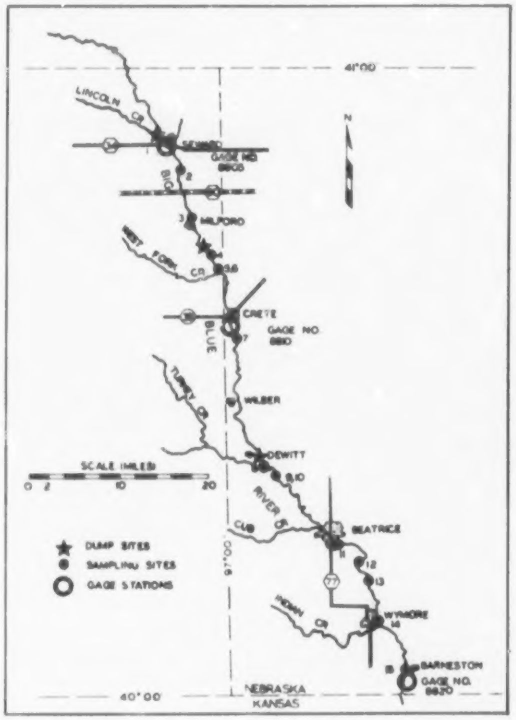

Fig. 1 Time-of-Travel Sampling Stations along the Big Blue River (Nebraska)

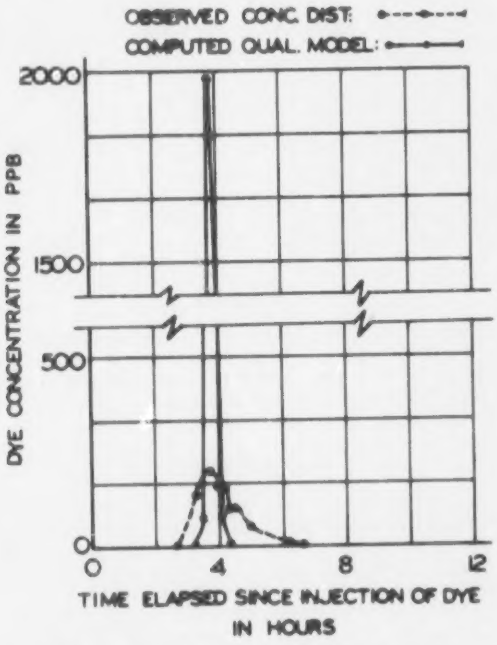

Fig. 3 QUAL-I Computed versus Measured Time-Concentration in the Big Blue River near Seward (Nebraska)

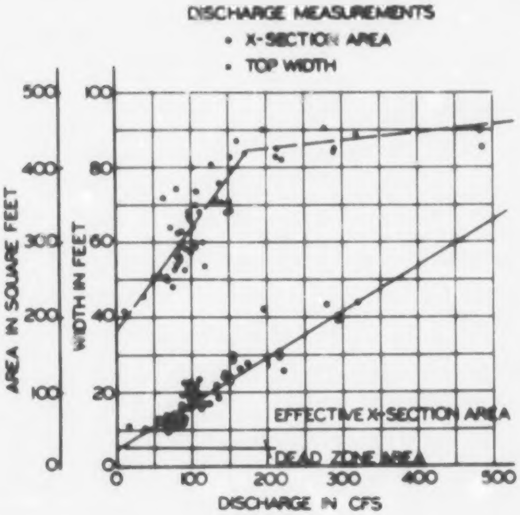

Fig. 2 Discharge Measurements on the Big Blue River near Crete (Nebraska)

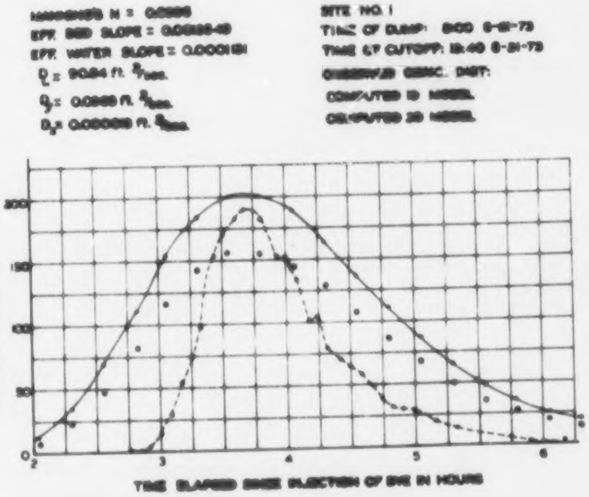

Fig. 4 Simulated versus Measured Time-Concentration in the Big Blue River near Seward (Nebraska)

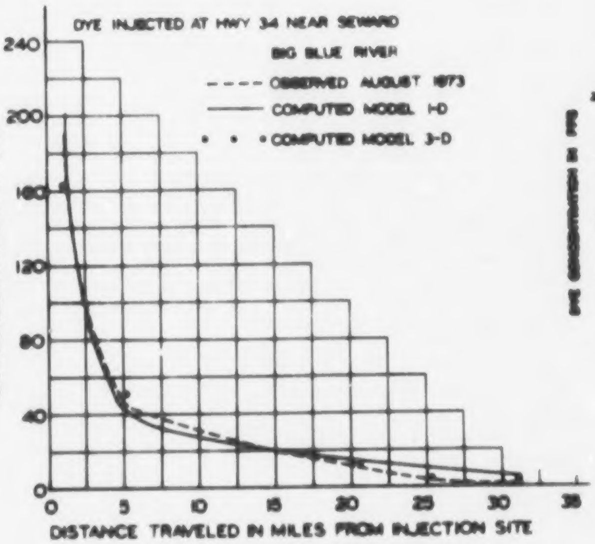

Fig. 5 Peak Concentration Variation in the Big Blue River between Seward and Crete (Nebraska)

SELECTING THE PROPER REAERATION COEFFICIENT FOR USE IN WATER QUALITY MODELS

Andrew P. Covar
Administrative Operations
Texas Water Quality Board
Austin, Texas

Abstract

Various methods for calculating atmospheric reaeration coefficients for use in mathematical water quality models are reviewed, and a rational engineering method is developed to guide the engineer in the selection of a proper predictive equation.

Introduction

The waste assimilation capacity for oxygen demanding materials of a body of water is primarily a function of three parameters; the volume of the water body, the allowable dissolved oxygen deficit, and the rate at which oxygen enters the water body from the atmosphere. The first two are simple concepts and are easily calculated, but the third, the reaeration coefficient, is more complex and more difficult to obtain. Many formulae have been developed for the water quality analyst to use in estimating this important coefficient, and in the past, it has been the practice to use whichever of these formulae produced the best "fit" to available dissolved oxygen data. While this may be an acceptable practice in some circumstances, it does leave the estimation of a very important parameter open to personal interpretation and bias. For this reason, a more objective method is suggested.

Review

Streeter and Phelps[1] (1925)

Streeter and Phelps in 1925 developed the classic oxygen sag equation for the prediction of the oxygen profile in a flowing stream. The equation was

$$\frac{dD}{dt} = K_1L - K_2D \qquad (1)$$

where dD/dt is the rate of change of the dissolved oxygen deficit, L is the amount of oxygen demanding material in the stream, D is the dissolved oxygen deficit, and K_1 and K_2 are the rate constants of decay and reaeration.

The prediction equation for K_2, the reaeration rate constant, was

$$K_2 = \frac{ZU^m}{(H')^2} \times 2.31 \qquad (2)$$

NOTE: (all equations give K_2 to the base e)

where U is the stream velocity, H' is the depth above minimum low water, Z is an irregularity factor, and m is a function of the mean change in velocity per change in gage height. Several of the variables in this expression must be empirically evaluated. This work did set the precedent for equations of this type and much of the subsequent research has been on the evaluation of constants to use in similar equations.

O'Connor-Dobbins[2] (1958)

This work was based on the theories of turbulent flow and the rate of renewal of saturated surface waters. A theoretical development was presented along with certain lab findings which tend to support some of the assumptions made. The predictive equation developed for streams displaying isotropic turbulence was

$$K_2 = \frac{(D_mU)^{0.5}}{H^{1.5}} \qquad (3)$$

where D_m is the molecular diffusion coefficient and H is the average stream depth. An additional equation was developed for streams with nonisotropic turbulence but O'Connor has since recommended using only the form shown. Based on field data reported by others and some rather rough estimates of system geometry, a comparison was made of reported values vs computed values. The authors reported good agreement.

Part of the criticism of their work has centered on the somewhat arbitrary manner in which they classified streams as isotropic vs nonisotropic. This is not significant in lieu of the O'Connor recommendation that only the "isotropic" equation be used. Other criticism involves some of the theoretical assumptions made in the development of the equation, and the estimates of stream geometry in the field area. Churchill, et al.[3] (1962) imply that the field data were for polluted streams which would interfere with verification. There is general agreement that the equation fairly accurately predicts reaeration coefficients for many different systems.

Churchill-Elmore-Buckingham[3] (1962)

This work was based on observed reaeration rates below dams from which oxygen-deficient water was released at a constant flow during the course of the experiment. This work is generally felt to be the most extensive and reliable set of field data available for the calculation of reaeration rates. Many different equations were tested and one important finding was that the reliability of the equation was not significantly improved by the addition of terms for slope, viscosity, surface tension, or any other of the many factors which could have an effect on the reaeration process. The equation suggested for use

$$K_2 = \frac{5.026\ U^{.969}}{H^{1.673}} \times 2.31 \qquad (4)$$

is of the same general form as the O'Connor-Dobbins equation.

Owens-Edwards-Gibbs[4] (1964)

This study involved the deaeration of six English streams with sodium sulfite and monitoring the oxygen recovery. Combining their data with that of Gameson, *et al.*[5] (1955) resulted in

$$K_2 = \frac{9.41\ U^{.67}}{H^{1.85}} \times 2.31 \qquad (5)$$

The streams involved in this study were generally less than 2.0 feet deep.

Langbien-Durum[6] (1967)

Langbien and Durum combined the field data of O'Connor and Dobbins (1958) and of Churchill, *et al.* (1962) with the lab data of Krenkel and Orlob (1963) and of Streeter, *et al.*[7] (1936) and obtained

$$K_2 = \frac{3.3\ U}{H^{1.33}} \times 2.31 \qquad (6)$$

Not all of Churchill's data were included in the analysis. The grouping of vastly dissimilar data to derive a single equation could be questioned. A better approach might have been to apply the separate equations only for stream conditions similar to those used in these derivation.

Isaacs-Gaudy[8] (1968)

Using a circular trough with recirculating water, a regression analysis on reaeration data yielded

$$K_2 = \frac{3.053\ U}{H^{1.5}} \times 2.31 \qquad (7)$$

The applicability of this equation has been criticized due to differences in stream flow characteristics in circular tanks and those found in natural streams.

Negulescu-Rojanski[9] (1969)

Similar to the work of Isaacs and Gaudy, this study involved a recirculating flume to yield

$$K = 4.74\ \left(\frac{U}{H}\right)^{.85} \qquad (8)$$

Due to the type of apparatus, the depths were limited to less than 0.5 feet.

Thackston-Krenkel-Orlob[10,11,12] (1963, 1966, 1969)

Much work has been done by these investigators using laboratory flumes and some field data. There is a lack of agreement among the various equations derived, and, as in similar work, the applicability of laboratory flume data to wider and deeper channels can be questioned. The reaeration process is clearly related to stream turbulence and similarities between turbulent flow in a laboratory flume and the turbulence in a more geometrically complex natural channel may not be as great as was assumed.

Tsivoglou[13,14] (1967, 1972)

Using a gas tracer technique developed in 1966, the author was able to directly measure the rate of gas transfer between a stream and the atmosphere. Tsivoglou concludes the "reaeration rate coefficient is directly proportional to the rate of energy expenditure in nontidal freshwater streams." In other words, K_2 equals the change in water elevation per unit time times some constant of proportionality. The equation suggested was

$$K_2 = 0.054\ \left(\frac{\Delta h}{t}\right) \text{ at } 25^{0}C \qquad (9)$$

with typical units for Δh and t being feet and days. Using 0.054 as the constant all the observed values for K_2 fell within ±50% of that value predicted by the equation. The author further concluded that flow changes by a factor of 2 or 3 do not significantly affect K_2. While the tracer technique offers the first reliable method for directly measuring the rate of gas transfer in natural streams, there was considerable "scatter" in the data.

Review Summary

In general, the laboratory studies involved flow regimes much different than those found in natural streams. These studies are useful in testing some of the conceptual models which strive to explain the reaeration process but their applicability to natural streams can be questioned. The investigators using field data used the best techniques available at that time to measure or estimate the reaeration coefficient. For a more detailed critique of previous work than has been presented here, see Lau[15] (1972) and Bennett and Rathbun[16] (1972).

A Suggested Method

The arbitrary selection of an equation to predict the reaeration coefficient can significantly bias the results of an analysis. This is illustrated in Figure 1. The only difference in the three dissolved oxygen sags shown is in the reaeration coefficient as predicted by the three equations suggested by O'Connor-Dobbins; Churchill, *et al.*; and Owens, *et al.* As you can see, the O'Connor-Dobbins curve predicts a minimum dissolved oxygen concentration of 5.0 mg/l while the Churchill, *et al.* curve predicts a minimum of 2.3 mg/l and a zone of dissolved oxygen less than 5.0 mg/l extending for 80 miles. It would obviously make a great deal of difference in an analysis which equation was used to predict this coefficient. Some of these differences might be eliminated given a good set of data and a proper calibration procedure but adequate data are frequently not available.

Of the several equations available to the water quality analyst, the two suggested by O'Connor and Dobbins and Churchill, *et al.* have much in their favor. The two equations are similar in form and have each been used extensively. Considerable effort was made to verify

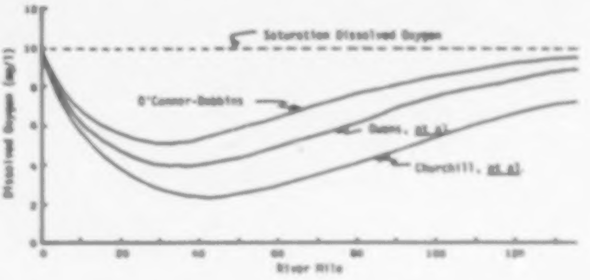

FIGURE 1. Effects of Different K_2 Equations on Dissolved Oxygen Sag

each with available data. Figure 2 illustrates the data used by O'Connor and Dobbins in the field verification of their equation and the data used by Churchill, et al. in their field work. Also shown is the data used by Owens, et al. in their work. It is evident that each equation was derived from or verified using streams with significantly different flow characteristics. There is very little overlap in the data. Since each of the authors cautioned against the use of their equation for streams with vastly different hydraulic characteristics, the figure has been divided into three regions each of which roughly includes most of the data used in one of the studies mentioned. The "A" line which divides the data of O'Connor and Dobbins from that of Churchill, et al. is also a line where the two equations suggested by these authors yield identical answers. The fact that this equivalence line separates the data so neatly tends to support the work of both groups. The "B" line was arbitrarily set at a depth equal to 2.0 feet to define the region containing most of the Owens, et al. data.

It is suggested that each of these three works cited is the most appropriate for combinations of depth and velocity similar to that used in the original research. For depths less than 2.0 feet, the equation suggested by Owens, et al. seems to have the strongest backing. For streams with depths greater than 2.0 feet, the selection of a proper equation would depend on which area of Figure 2 best describes the hydraulic properties of the stream in question.

The effect of such a selection method is shown in Figure 3. For each of the three areas, the reaeration coefficient has been calculated and plotted on the graph using the proper equation. Note the exact agreement between the O'Connor and Dobbins equation and the Churchill, et al. equation at all points along the upper line. There is fair agreement between the upper and lower areas of the graph at either end of the line drawn at a depth of 2.0 feet with progressively less agreement toward the center.

Conclusions

1. Much research has been done concerning the evaluation of the reaeration rate coefficient and its application to the field of water quality management.

2. With some notable exceptions there is generally poor agreement between the various equations derived.

3. Equations derived from very shallow laboratory flume data should not be applied to natural streams which probably have entirely different hydraulic characteristics.

4. Equations derived from field studies are best applied in instances where stream conditions are similar to those from which the equations were derived.

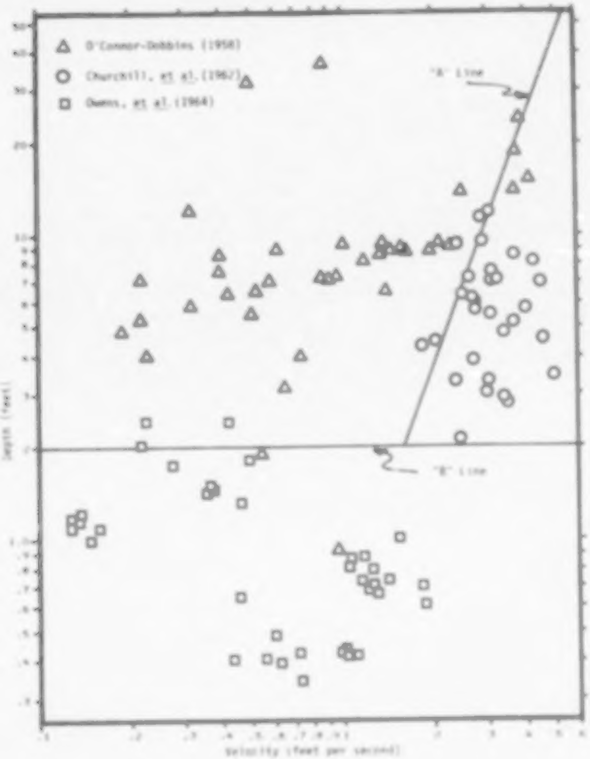

FIGURE 2 Field Data Considered By Three Different Investigators.

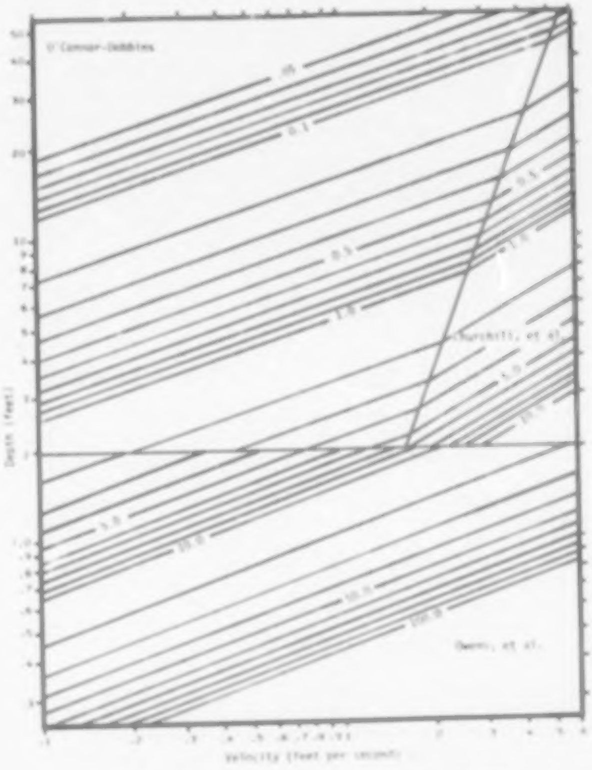

FIGURE 3 K_2 vs Depth and Velocity Using The Suggested Method.

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RECEIV-II, A GENERALIZED DYNAMIC PLANNING MODEL FOR WATER QUALITY MANAGEMENT

Charles V. Beckers, Peter E. Parker*, Richard N. Marshall and Stanley G. Chamberlain

Raytheon Company
Oceanographic and Environmental Services
Portsmouth, Rhode Island 02871

Introduction

Under funding by the US Environmental Protection Agency[1], Raytheon has developed the RECEIV-II Water Quantity and Quality Model[2]. In this paper, we discuss the background of the model development work and describe the model in some detail. To illustrate model applications, we present results from its use on the Pawtuxet River (RI)[3] and Norwalk Harbor (CT)[4]. We conclude the paper with a brief discussion of some of the apparent limitations of the model and areas in which improvements have already been made by Raytheon.

Background

The need for RECEIV-II stems primarily from Public Law 92-500, the Federal Water Pollution Control Act Amendments of 1972. Several sections of the law call for the states or their designated agencies to produce plans, commonly designated "303e" and "208" plans, for achievement of the stream water quality standards through selective application of discharge limitations and other institutional controls on the quality of water reaching the streams. In each case, accurate forecasting of stream quality is needed to determine the potential of the proposed plans for achieving these goals. Such forecasting is best done using computerized, mathematical models of water quality[5], allowing rapid assessment of expected water quality under rarely observed conditions, e.g. the 7-day, 10-year low flow.

Anticipating the need to produce such plans on a number of New England waterways, USEPA awarded Raytheon a contract to develop and calibrate water quality models for some 18 waterways in Rhode Island and Connecticut[1]. The calibrated models were to be capable of representing the following appropriately linked water quality constituents in each waterway:

- phosphorus
- coliforms
- ammonia nitrogen
- nitrite nitrogen
- nitrate nitrogen
- total nitrogen
- carbonaceous biochemical oxygen demand (BOD)
- chlorophyll a
- dissolved oxygen
- salinity
- a non-conservative metal ion to be selected by Raytheon.

While the waterways to be modeled are extremely diverse, ranging from upland streams through shallow lakes and impoundments to estuaries, it was concluded that overall project constraints could best be satisfied through use of a single, generalized set of coding. The generalized model had to be capable of representing the following basin features:

- Time-varying to handle tidal conditions and the chlorophyll a growth-death cycle.
- Two-dimensional to permit modeling the broad, vertically homogeneous areas of the vertically well-mixed estuaries.
- Multiple ocean inlets to cover such cases as New Haven Harbor and Narragansett Bay, where there are multiple inlets at the ocean boundary.
- Multiple shallow dams to deal with the multiplicity of mill ponds found on the New England rivers. (In the State of Rhode Island alone, there are nearly 400 dams, most dating from the nineteenth century textile industry.)
- Conservative and non-conservative constituents to handle the variety of water quality constituents considered in the project.

In addition, contractual clauses required that the models be capable of running on a variety of computers and of employing metric units.

Since no existing model satisfied all the requirements, it was decided to modify the Receiving Water Block (RECEIV) of the USEPA's Storm Water Management Model (SWMM)[6]. RECEIV was selected because it already included many of the necessary features, particularly the time-varying property, and could be straightforwardly modified to incorporate the others. It also had the incidental advantage of providing previously unavail-

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* Now at Institute of Paper Chemistry, 1043 East South River, Appleton, Wisconsin 54911.

able capability to SWMM. To clearly indicate its lineage, the new model was named RECEIV-II.

Description of RECEIV-II

RECEIV-II is a generalized, stand-alone model intended for use in forecasting water quality on a basin-wide scale, under alternative conditions of point and non-point discharge, stream flow and desired waterway usage. The emphasis is on forecasting the far-field effects of an individual discharge or assembly of discharges. Examples include the installation of additional treatment capacity at a municipal or industrial discharge, development of a new industrial site, population growth, institution of new zoning regulations, or establishment of a new control policy for flow regulation.

Fundamentally, RECEIV-II consists of two separate models coupled together. Hydraulic conditions are modeled first, using the QUANTITY section of RECEIV-II. Data on the temporal and spatial distribution of flow are then automatically transferred to the QUALITY section, in which water quality conditions are computed.

The analytical framework used to describe the waterway discretizes space and time, permitting numerical integration of the partial differential equations of hydrodynamics and water quality. The spatial framework uses the discrete element method[7] in which state variables such as surface elevation and constituent concentration are computed at nodes and transport (flow and velocity) is computed in channels linking the nodes. The temporal framework consists of discrete, uniform timesteps, with step duration selected independently in the QUANTITY and QUALITY sections. (For computational reasons, the QUALITY timestep must always be greater than or equal to the QUANTITY timestep.)

Fundamental Equations

The fundamental equations of the QUANTITY model are the reduced, one-dimensional form of the equation of motion for uniform, incompressible flow in the open channels between the nodes:

$$\frac{\partial v}{\partial t} = -v\frac{\partial v}{\partial x} - g\frac{\partial H}{\partial x} - F_f + F_w \qquad (1)$$

and the continuity equation expressing conservation of mass for an incompressible fluid in the open-topped nodes:

$$A\frac{\partial H}{\partial t} = -Q \qquad (2)$$

where:

v = velocity (m/s)

t = time (s)

x = distance along the channel (m)

H = water surface elevation referenced to datum plan of the model (m)

g = gravitational acceleration ($= 9.8\ \mathrm{m/s^2}$)

F_f = acceleration due to fluid resistance ($\mathrm{m/s^2}$)

F_w = acceleration due to wind stress ($\mathrm{m/s^2}$)

Q = the net flow out of the node ($\mathrm{m^3/s}$)

A = the surface area of the node ($\mathrm{m^2}$)

The acceleration due to fluid resistance is estimated by the Manning formula:

$$F_f = \frac{gn^2 v|v|}{R^{4/3}} \qquad (3)$$

where n = Manning's roughness factor ($\mathrm{s/m^{1/3}}$)

R = hydraulic radius (m)

The acceleration due to wind stress is estimated by the Ekman formula:

$$F_w = \frac{K}{R}\frac{\rho_a}{\rho_w} U^2 \cos \Psi \qquad (4)$$

where K = windstress coefficient (≈ 0.0026)

$\frac{\rho_a}{\rho_w}$ = ratio of air density to water density ($\approx 1.165 \cdot 10^{-3}$)

U = wind speed (m/s)

Ψ = angle between the wind direction an and the axis of the channel

The numerical technique used to integrate equations (1) and (2) is detailed in the RECEIV-II Documentation Report[3].

The fundamental form of the equations describing volumetric average water quality constituent concentration in a node is:

$$\frac{dC}{dt} = \frac{1}{V}\frac{dM}{dt} - \frac{M}{V^2}\frac{dV}{dt} \qquad (5)$$

where C = volumetric average constituent concentration (typically, $\mathrm{gm/m^3}$)

M = constituent mass in node (typically, gm)

V = volume of node ($\mathrm{m^3}$)

Equation (5) expresses the concept of conservation of mass in a control volume, frequently called a continuously stirred tank reactor (CSTR)[8]. The derivatives on the right can be evaluated in terms of the flows and constituent masses crossing the boundaries of the node, and in terms of the bio-chemical reactions taking place in the node:

$$\frac{dC}{dt} = \frac{1}{V}\left[\sum Q_j \; (C_j - C) + \sum Q_i \; (C_i - C) + \sum M_g - \sum M_d\right] \qquad (6)$$

where Q_j = flows entering node from upstream nodes (m^3/s)

Q_i = flows entering node from point and non-point sources (m^3/s)

C_j = concentration of constituent entering node from upstream nodes (typically, gm/m^3)

C_i = concentration of constituent entering node from point and non-point sources (typically, gm/m^3)

M_g = rate of constituent mass gained due to biological, physical or chemical processes in the node (typically, gm/s)

M_d = rate of constituent mass lost due to biological, physical or chemical processes in the node (typically, gm/s)

The interactions among the eleven water quality constituents modeled in RECEIV-II are presented in the ($\Sigma M_g + \Sigma M_d$) terms. For example, the rather complex interactions affecting the dissolved oxygen are formulated as:

$$\frac{1}{V}(\Sigma M_g - \Sigma M_d) = k_9(C^* - C_9) - k_7 C_7 - a_{9,4} k_4 C_4 - a_{9,5} k_5 C_5 + a_{9,8}(G_8 - D_8')C_8 - (b/R) \qquad (7)$$

where C_9 = nodal concentration of DO

C^* = saturation concentration of DO

k_9 = DO reaeration rate

C_7 = nodal concentration of carbonaceous BOD

k_7 = rate of oxidation of carbonaceous BOD

C_4 = nodal concentration of ammonia nitrogen

k_4 = rate of oxidation of ammonia nitrogen to nitrite nitrogen

$a_{9,4}$ = stoichiometric ratio of oxygen in nitrite

C_5 = nodal concentration of nitrite nitrogen

k_5 = rate of oxidation of nitrite nitrogen to nitrate nitrogen

$a_{9,5}$ = stoichiometric ratio of oxygen in nitrate

C_8 = nodal concentration of chlorophyll a

G_8 = "growth" rate of chlorophyll a

D_8' = adjusted "death" rate of chlorophyll a

$a_{9,8}$ = stoichiometric ratio of oxygen produced per unit "growth" of chlorophyll a.

b = benthic oxygen demand

All reaction rates (k's) are adjusted for the effects of temperature during computation. Equations for computation of BOD oxidation rate, DO surface reaeration, DO reaeration at dams, saturation DO and exchange at the tidal boundaries are detailed in the RECEIV-II Documentation Report[2] along with the numerical integration procedures used in the QUALITY section.

Program Structure

RECEIV-II is written in ANSI-standard FORTRAN[9] to assure inter-computer compatibility and has been successfully tested on the CDC 6700, CDC Cyber 73, IBM 370/155 and Honeywell 6000/60 computers. It consists of a main program and 14 subroutines that perform various computational, input and output functions. The program can be modularized to minimize the total computer memory requirements, with the QUANTITY and QUALITY sections typically loaded and run independently. Information transfer among the program modules is via mass storage, either mag tape or disk. The coding of RECEIV-II has been carefully structured to preserve compatibility with the present SWMM, but the two models have not yet been integrated.

Model Input and Output

In order to compute the primary model outputs, RECEIV-II requires a wide range of information on the river basin being modeled. Since the equations used in RECEIV-II constitute our concept of how the waterway "works", the data required by RECEIV-II would be required under any circumstances to provide an adequate description of the waterway. Table 1 summarizes the necessary input data, and characterizes it according to the spatial and temporal intensity needed.

The primary computational outputs of RECEIV-II are:

- Stage or tidal height at each node (m above datum)
- Flow in each channel (m^3/s)
- Velocity in each channel (m/s)
- Constituent concentration in each node (typically, mg/l)

The frequency of output for each of these results is under user control and an integer multiple of the basic timestep of the model.

TABLE 1. RECEIV-II DATA REQUIREMENTS.

DATA REQUIRED \ CHARACTERISTIC	INITIAL ESTIMATE	CONSTANT	EACH CHANGE	PERIODIC	BASIN-WIDE	GRID COORDINATE	SOURCE	NODE	CHANNEL	OCEAN NODE
GEOGRAPHICAL										
Source location		●						●		
Node location		●				●				
Node-channel connectivity		●						●	●	
Dam location		●						●		
Ocean interface location		●						●		
Surface area		●						●		
Bottom elevation		●						●	●	
Length		●							●	
Width		●							●	
METEOROLOGICAL										
Wind speed and direction		●			●					
Evaporation rate		●			●					
Precipitation rate			●		●					
HYDRAULIC										
Tidal height				●						●
Stage height	●							●		
Velocity	●								●	
Manning coefficient		●							●	
Dam height, width & shape		●						●		
Background flow		●						●		
WATER QUALITY										
Water temperature		●						●		
Temperature compensation coefficient		●			●					
Constituent concentration	●							●		
Background concentration		●						●		
Ocean concentration		●								●
Ocean exchange rate		●								●
Reaction rate		●						●		
Benthic oxygen demand		●						●		
Reaeration constants		●							●	
Sunrise		●			●					
Sunset		●			●					
Maximum light intensity		●			●					
Saturation light intensity		●			●					
Extinction coefficient		●			●					
Growth coefficient		●			●					
Respiration rate		●			●					
Michaelis-Menton constants		●			●					
Nutrient ratios		●			●					
Grazing rate		●			●					
SOURCE CONDITIONS										
Flow			●				●			
Constituent concentration (or mass rate)			●				●			

Results

Under the original USEPA funding, Raytheon calibrated RECEIV-II to 18 New England waterways, with varying degrees of success using the data available in 1973[10,11]. The calibration results ranged from good to unusuable, with streams and rivers typically turning our better than bays and harbors. In at least one case, the Quinnipiac River, state officials have used the Raytheon-calibrated model to develop 303e waste load allocations, with only minor updating to reflect more recent data. Load allocations on other rivers and harbors have subsequently been achieved using improved data bases.

Availability of data was invariably the single most important factor controlling the success of the calibration effort in each waterway. In several cases, we were unable to find the minimum two sets of data needed for calibration. The data on bays and harbors were substantially weaker than on streams and rivers. Despite the heavy use of the bays and harbors for navigation, basic data on tides and currents were noticeably absent. As discussed above, the data necessary to RECEIV-II calibration are fundamental to an understanding of the processes active in a waterway. Failure to develop adequate RECEIV-II calibrations for a number of the 18 waterways is indicative of the state of knowledge of those waterways.

Another factor contributing to difficulty in calibration is a fundamental limitation of the model in representing the stream bed as a rectangular channel. RECEIV was originally developed as a stormwater model, representing relatively high-flow conditions. In contrast, application of RECEIV-II in the context of 303e load allocations requires modeling of very low flow conditions. In many cases, the use of a rectangular channel approximation breaks down under low flow, due either to reduction in stream dimensions or separation of the flow due to stream bed bathymetry.

However, in those waterways for which sufficient data were available, RECEIV-II has performed quite well. The Quinnipiac River is one example, and Raytheon has recently completed preliminary waste load allocations using RECEIV-II on Norwalk Harbor and the Pawtuxet River, under contract to Connecticut and Rhode Island, respectively. In each case, additional refinement of the basic calibration was required to achieve satisfactory results. This was accomplished through additional data collection and detailed analysis of available data. The results of these two wasteload allocations illustrate the desirability of using a dynamic quantity and quality model for 303e planning.

Pawtuxet River

The preliminary results of the load allocation work on the Pawtuxet River illustrate the importance of nitrogenous oxygen demand in achieving water quality standards for rivers. A single unit of ammonia nitrogen discharged at the Cranston Treatment Plant (approximately 14.4 MGD) has the equivalent effect on dissolved oxygen at the Broad Street Dam of 5.5 units of carbonaceous BOD. While the necessary removal of carbonaceous BOD is thought to be achievable by Cranston's consulting engineers, there is concern for the ability to maintain the equivalent nitrogen allocation necessary to maintain water quality standards, especially during the colder months of the year when biological nitrification processes are difficult to maintain. For this reason, the dynamic capabilities of RECEIV-II have been exercised to determine the sensitivity of the Pawtuxet River to nitrogenous demand under varying flow and temperature conditions. It is of interest to note that, with respect to the total treatment plant-river system, winter conditions may turn out to be the "critical period" for maintenance of the water quality standards, not the summer months as commonly assumed.

Norwalk Harbor

A similar conclusion concerning the "critical period" has been reached in the case of Norwalk Harbor, but for entirely different reasons. Algal growth in Norwalk Harbor appears to play a major role in the oxygen cycle, especially as it affects the carbonaceous and nitrogenous BOD assimilation capacity. During cold, dry weather, algal oxygen production is sufficiently reduced to constitute the maximum restriction on total BOD discharged into the harbor. In cold, wet weather, higher nutrients loadings tend to be offset by increased algal oxygen production. While warm, wet weather is relatively non-restrictive on total BOD, it is most restrictive on carbonaceous BOD removal at the Norwalk STP. The dynamic features of RECEIV-II permit detailed analysis of each of these cases without the need to recalibrate the model for changing conditions. In addition to allowing study of the seasonal variations, RECEIV-II also allows confirmation of such details of the oxygen cycle as the early morning minimum, which results from algal respiration through the nighttime hours. Sensitivity analyses also indicate Norwalk Harbor dissolved oxygen levels to be very sensitive to variations in sunlight intensity, as might be expected from the strong dependency on algal population. A similarly strong dependency on tidal range is exhibited, due to reduced exchange with Long Island Sound during neap tides.

Discussion

Thus, when sufficient data are available to adequately describe the waterway, RECEIV-II has proven itself to be a useful and dependable approach to forecasting water quality. Its unique dynamic features have allowed the examination of aspects of water quality that might otherwise have escaped notice. Because of the dynamic formulation, it is preferred for application to estuaries, for use in cases of un-steady discharge (e.g. stormwater runoff), for extrapolation to low flow conditions, and for examination of seasonal, daily or tidal variations in water quality.

As with all models, experience in the use of RECEIV-II has highlighted areas in which the model can be improved. When those improvements have related to features of the model developed under USEPA contract, Raytheon has publicized corrections and changes through release of Program Modification announcements. The objective is to assure the integrity of Raytheon's model in its use by the many agencies and firms now holding copies. To date, nine Program Modifications have been distributed to the user group through the USEPA.

In addition, Raytheon has found it necessary to further expand the model's capability beyond that originally required for RECEIV-II. To satisfy various contractual commitments, Raytheon has developed the proprietary RECEIV-III model. Among the numerous improvements incorporated in RECEIV-III are coding to model water temperature and organic nitrogen (coupled to chlorophyll a and ammonia nitrogen).

Beyond the improvements discussed above, there are several areas in which RECEIV-II may still be improved. Incorporation of RECEIV-II (or RECEIV-III) into SWMM remains a highly desirable, but non-trivial, goal. RECEIV-II is designed to represent the complex interactions among eleven water quality constituents, while SWMM has capacity for only six of the classical BOD-DO form. Similarly, removal of the rectangular cross-section limitation described above is highly desirable, perhaps by substitution of a more flexible parabolic cross-section. Again, such a change is non-trivial, since it goes to the heart of the QUANTITY model formulation. Nonetheless, we recommend both these improvements as being well worth the effort

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MODIFICATIONS TO QUAL - II TO

EVALUATE WASTEWATER STORAGE

John S. Tapp
Technical Support Branch
Water Division
EPA, Region IV
Atlanta, Georgia

Summary

To help evaluate the feasibility of storing wastewater to alleviate adverse effects on receiving water quality during low flow conditions, the water quality model QUAL - II was modified. The general modifications are described and situations which lend themselves to application of the modified model are discussed.

Introduction

Effluent limitations for wastewater discharges are commonly established based on maximum temperature at some critical statistical low stream flow condition, normally defined by water quality standards. Thus, commonly utilized procedures of arriving at effluent limitations based on water quality standards in some situations do not take into account, (a) water temperature changes, (b) flow rate fluctuations, or (c) other seasonal variations. For situations where assimilative capacity is limited and the storage of effluent from a wastewater treatment facility is feasible, the normal seasonal changes in water temperature and flow rates can be utilized to allow instream water quality standards to be maintained, at a cost less than by utilizing treatment alone. Under extremely critical conditions, even the possibility of no discharge could be investigated.

To use the wastewater storage approach requires curves of stream flow versus wastewater flow at a given quality to maintain some instream constituent concentration, generally dissolved oxygen. To establish the curves of stream flow and allowable wastewater flow, a mathematical model is very useful. However, most dissolved oxygen models are not constructed such that these curves can be determined without much trial and error input and manipulation. This paper describes the modifications to a commonly used model to allow easy generation, without trial and error manipulation, of curves of stream flow versus wastewater flow (at a given oxygen demand concentration) to maintain a given instream dissolved oxygen concentration.

The Model

The model selected for modification was QUAL - II as developed by Water Resources Engineers[1]. QUAL-II is a modification of QUAL - I originally developed for the Texas Water Quality Board. As developed, QUAL-II can simulate the dynamic behavior of conservative materials; temperature; carbonaceous biochemical oxygen demand; chlorophyll A; the nitrogen forms of ammonia, nitrite, and nitrate; phosphorus; benthic oxygen demand; dissolved oxygen; and coliforms. All constituents except temperature can also be simulated directly in the steady state mode. The general model constituent layout is shown in Figure 1.

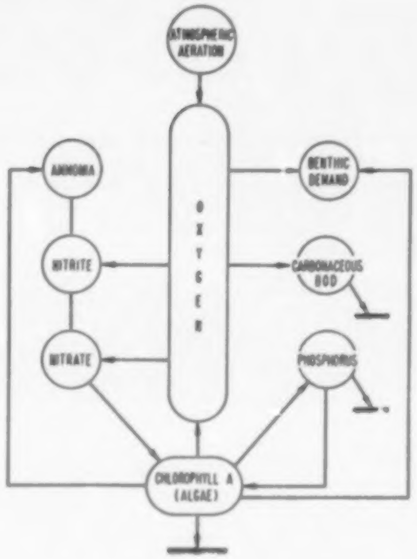

Figure 1
The General Model Constituent Layout for QUAL-II

QUAL - II is structed as one main program supported by 19 subroutines. The general structure of the model is shown in Figure 2. The description of the various subroutines and their functions are described by Water Resources Engineers[1] and need not be repeated here. The main focus of the modifications to QUAL-II was to take advantage of subroutine FLOAUG to check for a prespecified instream dissolved oxygen target level. If that level was not met all flows would be incrementally increased based on drainage area contribution to arrive at a flow in a prespecified headwater which would allow the dissolved oxygen target to be met in all reaches below the discharge under study. All data necessary to utilize the modified model is read in subroutine INDATA and model control is maintained by the main program QUAL - II.

The detailed modifications made to QUAL-II are described by Tapp[2]. Basically, the model was modified such that a drainage area and a drainage area factor would be assigned to each reach, to each direct input tributary, and to each headwater. A range of wastewater flows for the specific discharge to be studied is specified. For a given wastewater flow the model uses subroutine FLOAUG to check for a minimum instream dissolved oxygen concentration. If the dissolved oxygen concentration is less than the minimum, then subroutine FLOAUG increases the flow in each reach, direct input tributary, and headwater in proportion to the drainage area and drainage area factor. When the dissolved oxygen concentration below the discharger under study is above the specified minimum, the sequence returns to the main program where a new wastewater flow is taken through the same procedure. The output from the model is a series of wastewater flows with corresponding stream flows for the headwater above the discharger under study at a given temperature and given wastewater effluent quality. The modifications were developed for the steady state mode and have not been tested in the dynamic mode.

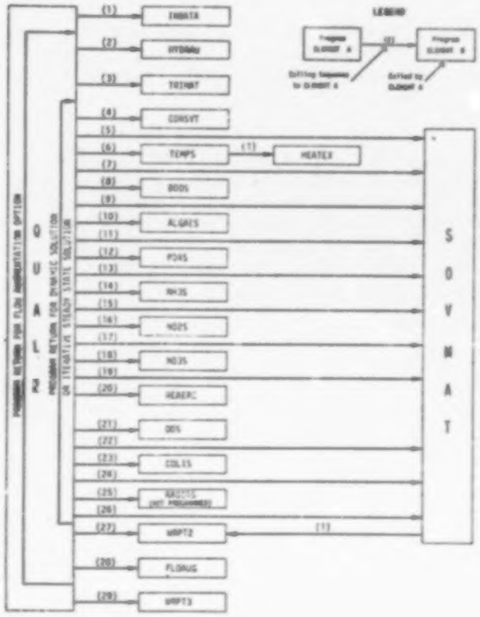

Figure 2
The General Model Structure of QUAL - II

Model Utility

The type of curve which can be plotted from the information developed by the modified QUAL-II model is shown in Figure 3. For any stream flow in the headwater above the discharger under study, an allowable wastewater flow to meet a given dissolved oxygen target level can be determined at a given stream temperature and effluent quality. Knowing the hydrology of the headwater above the discharge, the storage volume necessary to maintain the dissolved oxygen target can be determined. This can be accomplished for a discharger and a given effluent quality by generating a curve of wastewater flow versus stream flow to meet a given instream dissolved oxygen concentration for the water temperature associated with each month of stream flow records. A temperature simulation model based on meterological data could be linked with the hydrologic data to provide daily water temperatures, if desired. Knowing the water temperature and a daily stream flow value, one could go to the wastewater flow versus stream flow curve for that temperature and effluent concentration and arrive at an allowable wastewater flow. The average daily flow of the discharger would then be compared with the allowable wastewater flow and if the flow from the discharger was greater than the allowable flow the difference would be put into storage. If the discharger flow was less than the allowable flow then the difference would be taken from storage and put into the stream along with the flow from the discharger. For the period of hydrologic records under evaluation, this procedure could be utilized to arrive at the maximum storage volume required for the given effluent quality and would be one point on a storage volume versus effluent quality curve. Where large amounts of hydrologic records are to be utilized the wastewater flow versus stream flow curves can be defined by fitted equations and a curve at one temperature can be related to a curve at another temperature by the use of temperature coefficients. Once these relationships are established the storage volume can easily be calculated by simple digital computer routines.

Utilizing the above procedure, other storage volumes are then determined for varying effluent concentrations and a curve of effluent quality as measured by ultimate oxygen demand (UOD) versus the storage volume necessary to maintain a given instream dissolved oxygen level can be determined as shown in Figure 4. From the information of oxygen demand in the effluent versus storage volume, costs of wastewater treatment and storage costs can be used to develop the curves shown in Figure 5. The minimum point on the total cost curve would give the least cost combination of storage and treatment.

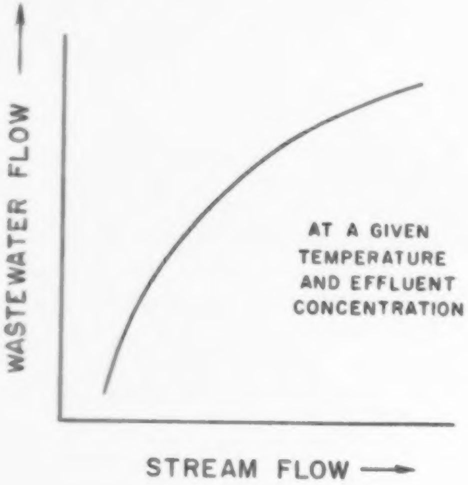

Figure 3
An Example of the Curve Which Can be Plotted from Points Generated by the Modified QUAL-II Model

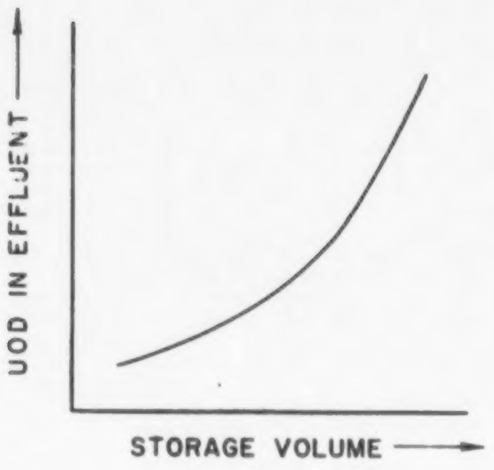

Figure 4
A Curve of Oxygen Demand in the Effluent Versus Storage Volume

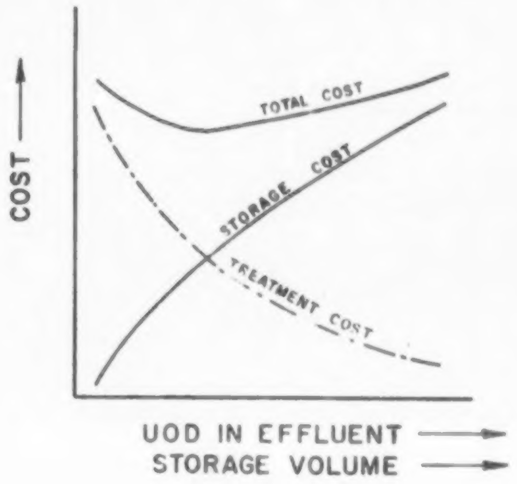

Figure 5
The Curves Showing the Least Cost Combination of Storage and Treatment

Another example where the modified QUAL-II model could prove useful would be a situation where instream dissolved oxygen standards could not be met with an industry discharging at an effluent quality defined as Best Available Treatment (BAT). In this instance, effluent concentration would be left constant and storage volumes tested against allowable instream dissolved oxygen concentrations. A study of this type was conducted by Tapp[3] where the curves of allowable wastewater flow versus stream flow were developed by trial and error, thus pointing to the need for the modified model. In this study an industry which was the definition of BAT for its class had an existing storage pond of a given volume. An idea of what instream dissolved oxygen concentration could be maintained based on over 30 years of past hydrologic records on the stream was desired. A curve of allowable wastewater flow versus stream flow for each average monthly water temperature was plotted and broken into two sections each fitted by a straight line with a slope and a Y-intercept. The slopes and Y-intercepts at different temperatures were related by coefficients such that for each instream dissolved oxygen level investigated the allowable wastewater flow was only a function of the stream flow and the temperature. A digital computer program was written to read in over 30 years of stream flow records, assign the proper temperature, and calculate and accumulate the storage volume of wastewater. Based on this output, an equation for operation of the storage pond to meet the required instream dissolved oxygen concentration was developed.

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WATER POLLUTION MODELING IN THE DETROIT METROPOLITAN AREA

Michael Selak
Robert Skrentner, P.E.
City of Detroit
Detroit Water and Sewerage Dept.
Detroit, Michigan

Carl Harlow
James Anderson, P.E.
College of Engineering
Wayne State University
Detroit, Michigan

SUMMARY

The EPA Storm Water Management Model (SWMM) has been used by the Detroit Water and Sewerage Department and Wayne State University to simulate waste water flow in the Oakwood Sewer District of the City of Detroit. This District is a 1,500-acre (3,705-hectares) residential/industrial area with combined sewers from which flow is pumped to the Detroit waste water treatment plant and/or to the Rouge River during periods of high rainfall. After several minor modifications to the SWMM, the simulation results from the Runoff and Transport blocks of SWMM compared favorably with observations by the computerized monitoring system of the Detroit Water and Sewerage Department.

The output from the SWMM Transport block is routed to a computer simulation of the Detroit waste water treatment plant called STPSIM, which was developed at Wayne State University. This model enables the user to evaluate the effect of storm flow on plant performance and to compare various strategies for treating the stored waste water. The simulated results from STPSIM appear to be quite representative of the actual treatment plant performance. However, model calibration has been difficult due to a shortage of real-time data from the plant.

All of the water pollution simulation models operate on Wayne State University's 360/67 computer system in time sharing or batch mode through an executive program called the Detroit Water Quality Information System (DWQIS). The DWQIS was developed at Wayne State University with assistance from the Detroit Water and Sewerage Department. In addition to the above models, the DWQIS contains census and local climatological data for the Detroit area which was used to provide some of the necessary input data for the SWMM.

INTRODUCTION

Ninety-seven communities of the Detroit metropolitan area are supplied with potable water and seventy-four communities receive waste water collection and treatment services from the Detroit Water and Sewerage Department (DWSD). As of July 1975, the waste water service area under DWSD contract was 1075 square miles (2784 sq. km.). The collection system contains separate sanitary and combined sewers that normally flow to the DWSD regional treatment plant located at the confluence of the Detroit and Rouge Rivers. This plant provides advanced secondary treatment to a flow of 450 million gallons per day (19.7 cms). Total plant flow averages 800 MGD (35.0 cms). Seventy-six possible points of overflow to the Detroit and Rouge Rivers exist to relieve the system during periods of extreme flow. The plant is currently undergoing a major improvement program including the installation of a computer system that will monitor and aid in the control of the treatment unit processes.

The DWSD, with an EPA research and demonstration grant, installed a system-monitoring and remote control network to better integrate the waste water collection and treatment operations. The data collected by the network is transmitted to the DWSD System Control Center and provides operators with information to remotely control dry weather and storm pump stations, flow regulating devices, inflatable dams, and the entire water distribution network. The DWSD computers monitor events as they occur, but they are not capable of predicting system response to storm events and the resulting changes in waste water quality and quantity. For these reasons, the DWSD has begun a program of utilizing computer models to predict system behavior, which is a primary goal for optimizing the performance of an existing system. The objective of the DWSD is to implement methods that will provide system response information in an attempt to utilize the storage capabilities of the sewer system more efficiently, improve upon the system operation to prevent overflows, and operate the treatment plant more efficiently. To meet these objectives, the DWSD is applying the EPA model SWMM and the Wayne State University treatment plant simulation model STPSIM to the Detroit system.

APPLICATION OF SWMM TO THE OAKWOOD SEWER DISTRICT

The Oakwood Sewer District of the City of Detroit was selected to test and evaluate SWMM because: a) it is relatively isolated from the balance of Detroit, b) its land use is typical of the City, and c) it is of a manageable size. The district has a population of 17,250 and an area of 1500 acres (607.5 hectares). 46% of the land area is classified as residential, 44% as industrial, 3% as commercial, and 7% parkland. A combined sewer system collects and transports sanitary flow, industrial wastes, and storm water to a single pump station. Under normal conditions, a 20.0 cfs (0.6 cms) pump transports the dry weather flow to the main plant. During periods of high flow due to storm water, additional pumps with a total capacity of up to 488 cfs (13.8 cms) can be used to relieve the system into the Rouge River near its confluence with the Detroit River. As part of the system-monitoring network, the pump station is equipped with a weighing bucket and a tipping bucket rain gage. An additional tipping bucket rain gage is located in the near vicinity. In addition, three level sensors are operating in the major sewers of the district. During periods of rainfall, the system-monitoring network is capable of collecting rainfall data with time intervals as small as five minutes. The level sensors provide flow data on a continuous basis.

The major blocks of the SWMM that were utilized in this study include RUNOFF, Version I and TRANSPORT, Version II. Version II of the RUNOFF block is currently being evaluated. The dual-stage pump capacity built into the TRANSPORT block was found to be inadequate for the conditions at Oakwood and had to be modified to allow for multiple pumps of different capacities. Several storms with rainfalls of up to 2 inches extending over 40 hours were used to evaluate the models.

RUNOFF BLOCK

The Oakwood district was initially divided into 150 subcatchments with an average size of 10 acres (4.05 hectares). Land use divisions, sewer maps, U. S. Census data, previous DWSD reports, and topographic maps all played an important role in this selection process. Pipes up to 24 inches (61 cm.) in diameter were included in the RUNOFF block. Due to the long computer times needed for this configuration, later analyses used as few as 50 subcatchments of up to 80 acres. Storm durations ranged from 3 to 40 hours with a maximum of 120 time steps of 15 minutes used for the 40-hour storm. Although this is in excess of the SWMM recommendations, it was about the smallest that could be used without altering the RUNOFF block, and no serious difficulties were encountered.

TRANSPORT BLOCK

The output from RUNOFF becomes the input to the TRANSPORT block. The combined sewers of the Oakwood district are circular or egg-shaped, monolithic concrete or brick, and range in diameter from 3 to 10 feet (.92 - 3.05 meters). Most of the necessary input data for this block was taken from DWSD sewer maps, the U. S. Census, and DWSD water use data. The major sewers were divided into 138 elements, and as in RUNOFF, 120 time steps of 15 minutes each were used for the simulation. The Oakwood pump station has four pairs of pumps with capacities of 20 cfs (0.6 cms), 40 cfs (1.1 cms), 98 cfs (2.8 cms), and 106 cfs (3.0 cms), respectively. Under normal conditions, one 20-cfs (0.6-cms) pump handles dry weather flow. As the level in the wet well rises, additional pumps are activated as needed. For the storms modeled in this study, the 20-cfs (0.6-cms) pump handled dry weather flow and two 40-cfs (1.1-cms) pumps were used during the overflow condition.

The dry weather flow, infiltration, inflow, and insystem storage option of TRANSPORT were used in this study, but the insystem storage model was found to be inadequate for the conditions in Oakwood. Consequently, DWSD computer programs were used to determine the storage potential of the Oakwood sewers which was then utilized in TRANSPORT as an "irregular reservoir".

SWMM RESULTS

In general, the results generated by SWMM correlate satisfactorily with observations and it seems that SWMM is capable of predicting the waste water system behavior. Figure 1 shows the relationship between the rainfall hyetograph and the resulting runoff hydrograph. No data was collected to verify this relationship, but the pattern is clearly representative. Figure 2 is a plot of the actual and simulated overflow from the Oakwood pump station.

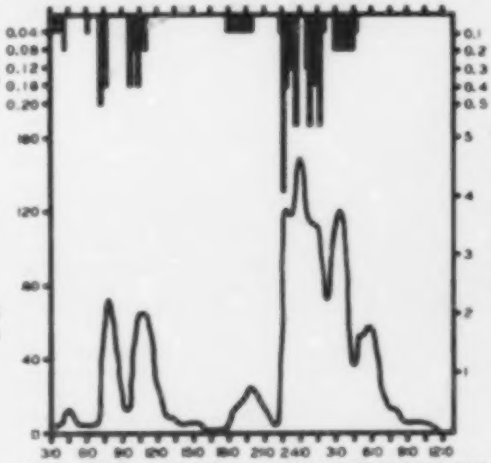

FIGURE 1-RAINFALL HYETOGRAPH & RUNOFF HYDROGRAPH VS. TIME

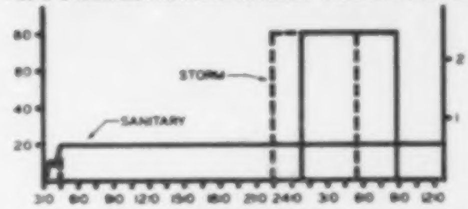

FIGURE 2-PUMP FLOW VS. TIME
SOLID-MODEL DASHED-REAL

The quantity of waste water that overflowed was predicted within the accuracy of the measured data. However, the time that the pump was predicted to have gone on deviated from the actual pump records by approximately two hours. Based on an elapsed time of 20 hours from the beginning of the simulation, this represents a deviation of approximately 10%. Considering the accuracy of the input data and the state-of-the-art of the models, this deviation seems quite reasonable.

WASTE WATER TREATMENT PLANT SIMULATION

STPSIM is a dynamic waste water treatment plant model which uses the digital computer to simulate plant behavior. The computer program is written in Fortran and consists of various subroutines totaling approximately 1500 lines. STPSIM currently has the capability of modeling; 1) settleable solids, 2) suspended solids, 3) dissolved solids, 4) B.O.D., and 5) chlorides. The output from STPSIM is displayed in tabular and graphical forms with the graphical display being optional. Through STPSIM, the user can study plant behavior by adjusting various operation parameters such as tanks in service, recycling, chemical feeds, etc.

There are many reasons for studying the dynamic behavior and operational characteristics of wastewater treatment processes, including optimizing the treatment of processes by properly adjusting operational controls. Some of the possible benefits that could be derived from this optimization are:

1. Reduced costs: savings on chemicals and electrical energy.
2. Better treatment of dry weather flow: higher removal efficiencies might be obtainable during normal plant operation.
3. Higher treatment capacities: through better control it might be possible to treat higher capacities during high runoff periods while maintaining water quality standards.

A dynamic model is needed since waste water treatment systems are rarely at steady-state due to significant variations in flow quantity and quality during a given day (1). This can be seen in Figure 3 where the concentration of suspended solids of the influent was measured hourly for the Detroit waste water treatment plant on February 23 and 24, 1975.

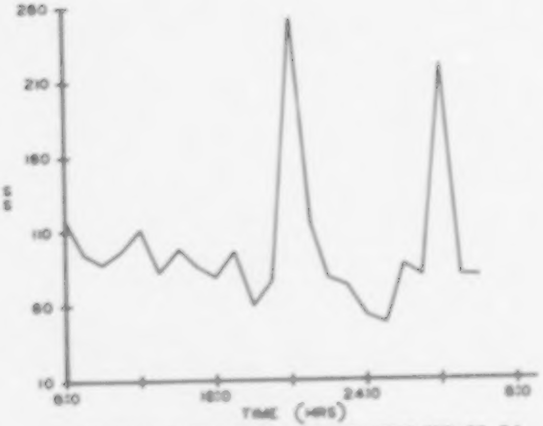

FIGURE 3-OBSERVED PLANT INFLUENT FEB. 23-24 (SS-SUSPENDED SOLIDS, MG/L)

However, treatment processes are usually operated as steady-state systems with general operating procedures based on flow quantity rather than flow quality. Furthermore, to report the efficiency of a given process, the samples are usually extracted from the inlet and the outlet at approximately the same time. This obviously assumes that the process is at steady state.

STPSIM REQUIRED INPUT DATA

STPSIM requires the following types of information:

1. Time information: time step and length of analysis.
2. Quality information: influent concentrations for the pollutants that will be analyzed for each time period.
3. Quantity information: flow rates for each time period.
4. Plant operating information: which tanks will be in service, initial concentrations of tanks, routing schemes, recycle schemes.
5. Calibration information: (optional) reaction coefficients, reactor behavior type.
6. Desired output: graphical, tabular, or both.

The quality and quantity data can be the output from the TRANSPORT block of SWMM or from plant observations.

BASIC ALGORITHM

The basic reactor type used for modeling the various processes is the "complete mixed" reactor. Some of the processes act as plug flow reactors while others have complete mix characteristics (5). Plug flow is usually approximated in long tanks with a high length-to-width ratio in which longitudinal dispersion is absent or at least minimal. This condition is usually characteristic of primary sedimentation tanks. Complete mixing occurs when the pollutant entering the tank is immediately dispersed throughout the tank. Round or square tanks are generally representative of this condition. Aeration tanks, for the activated sludge process are usually operated under complete mix conditions (1,7). However, in many instances, the reactors cannot be properly characterized by either of the above ideal types and therefore are classified as non-ideal reactors.

The complete mix reactor was chosen as the basic reactor for STPSIM since it is possible to model plug flow and non-ideal reactors with this model in parallel and series combinations.

For a single complete mix reactor, a mass balance yields, for a given time,

Mass in = Mass out + Disappearance by reaction + Accumulation

$QC_{in} = QC + RV + V\,(dC/dt)$ where

Q = flow - constant for a given tank
V = volume of the tank, constant over time
C = concentration of pollutant in tank
C_{in} = incoming concentration of pollutant

R = reaction mechanism
t = time

This basic differential equation is solved numerically at each time step for each pollutant and for each reactor.

The various reactor types are handled in the following manner:

1. Complete Mix - use of the basic algorithm
2. Plug Flow - use of "N" complete mix subreactors in series. As "N" approaches infinity, the behavior will approach that of plug flow, Figure 4.

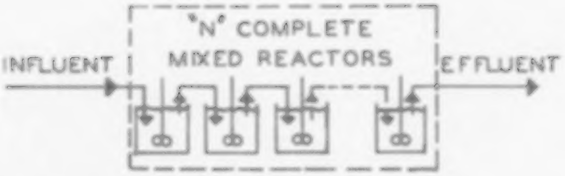

FIGURE 4 - PLUG FLOW REACTOR

3. Non-ideal types - using complete mix (CM) and plug flow (PF) reactors in parallel and series combinations along with recycle schemes, Figure 5.

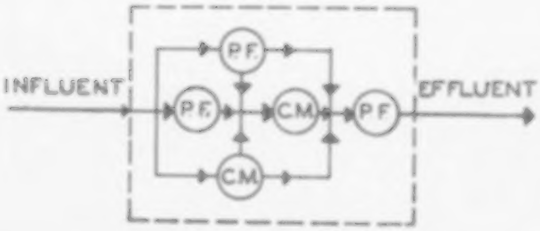

FIGURE 5 - NON-IDEAL REACTOR

RESULTS

STPSIM has been used to model the Detroit Waste Water Treatment Plant. The analysis chosen for presentation is for suspended solids for the 23rd and 24th of February, 1975. Suspended solids were measured on an hourly basis during this period for plant influent and effluent. On this date, the activated sludge system was not in operation which permitted the sedimentation processes to be modeled alone. If the activated sludge system had been in operation, additional information would have been required. As seen in Figure 6, there appear to be questionable data points for the effluent measured at 2:00 P.M. on the 23rd and at 4:00 A.M. on the 24th. The approximate residence times during this period were on the order of one hour. Therefore, if peaks in the effluent did occur, similar peaks should have existed in the influent earlier, but none were observed.

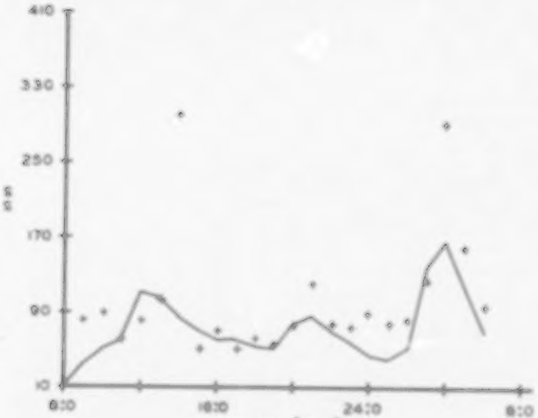

FIGURE 6 - SIMULATED & OBSERVED (+) PLANT EFFLUENT FEB. 23-24 (SS - SUSPENDED SOLIDS, MG/L)

Several possible explanations exist. One is that the measured points are in error, which is impossible to check at this time. A second explanation might be that the measured effluent points were correct and internal operations, such as recycling, were responsible. However, this information also was not available. Finally, a third explanation could be that the influent peaks did occur prior to the effluent peaks, but were missed. This alternative is examined below.

For this analysis, two influent points were adjusted to creat 'artificial' influent peaks prior to the two effluent peaks in question. The measured influent at 12:00 P.M. on the 23rd was changed from 100 mg/l to 270 mg/l and the measured influent at 3:00 A.M. on the 24th was changed from 90 mg/l to 320 mg/l. All tanks in operation, which were basically sedimentation tanks, were modeled as plug flow reactors. Initial suspended solids concentrations for all reactors were assumed to be 10 mg/l.

It appears, by observing Figure 6, that the initial concentrations were set too low and that it took approximately three hours before simulated values agree with measured values. From this time until about 12 hours later, simulated values agree reasonably well with observed data. This period of agreement was also evidenced in other analyses of this same data where adjustments in the influent points were not made. An interesting point is that these artificial influent peaks were still unable to explain the 'questioned' effluent peaks, and the correlation of observed with simulated concentrations was [illegible]. Therefore, it appears either that these effluent peaks did not occur, or that internal operations were responsible.

As additional plant operating data becomes available, it should be possible to calibrate STPSIM for other pollutants over a range of flow conditions. These preliminary results indicate that STPSIM can be developed to the point where it will be a useful tool for operating the plant.

DETROIT WATER QUALITY INFORMATION SYSTEM

The efficient use of all of these models, especially if real-time plant operating information is expected in a short time frame, requires a relatively sophisticated computer management system that provides for easy access to, and updating of, the input data along with assignment of I/O devices and proper sequencing of the programs. The Detroit Water Quality Information System (DWQIS) is a time sharing/batch mode Fortran program designed to meet these needs. In addition to SWMM, STORM, and STPSIM, the DWQIS manages the execution of the Wayne State University Air Quality Information System (AQIS) and the Detroit Metropolitan Area Data System (DMADS). Efforts are currently underway to use the air pollution simulation data as input to SWMM-RUNOFF to determine the effect of air pollution washout on water quality. The data system, DMADS, provides much of the socio-economic input data for SWMM and STORM. The DWQIS also stores, retrieves and updates data files on disc and tape, using language familiar to engineers and technicians. A program to check for probable errors in the input data for the various models is also being implemented as part of the DWQIS. These features are very important if a large staff of people with or without strong computer capabilities are to be working on the project.

MANAGEMENT AND MODELING

Based on DWSD's experience with the Oakwood sewer district, modeling costs for overflow quantity could range up to $3 - $5 per acre ($1.2 - $2.0 per hectare) depending on the accuracy required. These costs include salary, fringe benefits, overhead, and computer time. Sampling costs are expected to be a maximum of $15,000 per outfall for a detailed sampling program to obtain data for diurnal and seasonal variations in quality for dry and wet weather flow. Total sampling costs will also depend on the desired model accuracy, quality variations among outfalls, and sampled parameters. For the wastewater treatment plant, a $30,000 to $50,000 sampling program should provide sufficient model calibration data. The estimated total modeling cost is about 0.25% of the DWSD's estimated overflow abatement and plant expansion construction costs through the year 1990.

As more overflow abatement facilities are added to the system, a means must be found to operate the system in a more coordinated and efficient manner. Because of the large number of potential operational modes, computerized analysis is perhaps the only viable alternative to optimize waste water collection system operations. System response model output could provide the input data to the optimization models. Modeling of the treatment plant will allow for alternative modes of operation to be simulated. Considering that DWSD treatment plant chemical and utility costs for 1975 exceeded $6 million, an increase in operational efficiency of as little as 1% or 2% could easily justify the cost of modeling.

Since environmental modeling and simulation is a relatively new tool available to assist managers in decision making related to the planning, design, and operation of their systems, its use is limited. To encourage the expanded use of modeling techniques, it is recommended that a series of mini-seminars be held with EPA sponsorship to explain the ramifications of modeling to managers. The seminars should stress the anticipated costs of modeling and the expected benefits.

It is further recommended that additional EPA funds be committed to research and demonstration grant projects related to modeling and to improving the state of the art in both waste water sampling and flow measurement. These funds should be at least 0.5% of the monies committed for construction grants. In addition, the grants should be 100% federally funded for projects which will utilize models or measurement devices within urban watersheds and in conjunction with the municipalities or agencies having jurisdiction over the waste water system.

In summary, modeling appears to be a viable means to analyze waste water collection/treatment systems. Thus, a major objective of EPA must be to encourage model development, usage, and calibration.

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GENERALIZED METHOD FOR EVALUATING
URBAN STORM WATER QUALITY MANAGEMENT STORAGE/TREATMENT ALTERNATIVES

James P. Heaney, Wayne C. Huber and Sheikh M. Hasan
Department of Environmental Engineering Sciences
University of Florida
Gainesville, Florida 32611

Michael P. Murphy
William M. Bishop, Consulting Engineers
Tallahassee, Florida 32302

Summary

We are nearing completion of an EPA-sponsored study in conjunction with the American Public Works Association to estimate the nationwide cost of controlling pollution from combined sewer overflows and storm sewer runoff.[1] Two models, the USEPA Storm Water Management Model (SWMM) and the Corps of Engineers' STORM, were used extensively in this study to estimate pollutant loading rates and evaluate various storage/treatment alternatives.[2 3 4] Detailed modeling studies were performed in Atlanta, Denver, Minneapolis, San Francisco, and Washington, DC. This paper describes the results of continuous simulation of hourly rainfall and runoff in these cities for a wide variety of assumed availabilities of storage and treatment combinations. Results of these simulation studies are presented as isoquants showing the technologically efficient combinations of storage and treatment to obtain a specified per cent pollution control. This information is combined with cost data developed in this study to determine the optimal combination of storage and treatment for any desired level of control for each of the five cities. The results are presented in a normalized form which enables engineers and planners to derive preliminary estimates of control costs for other cities. This information is useful for early phases of 208 planning and for NEEDS surveys. A more complete description of this procedure is presented elsewhere.[5]

Simplifying Assumptions

In order to devise such a general procedure, numerous simplifying assumptions were made. A constant per cent BOD removal was assumed for the treatment units. In actuality, performance would vary widely due to the dynamic nature of the inflows. No account is taken of the equalizing effects and treatment which occur in storage. Cost functions are based on relatively few actual installations. The tradeoff between treatment plant size and pipelines is not considered explicitly. Approximate curves fit to the results for the five cities are extrapolated to the other 243 urbanized areas.

Multipurpose waste management schemes are not considered. Actual costs for a given city could be quite different than the estimates obtained using this highly simplified procedure. However, the methodology is general. Thus, the user needs only to substitute more accurate local data to obtain refined estimates.

Control Technology and Associated Costs

A wide variety of control alternatives are available for improving the quality of wet weather flows.[6 7 8] Rooftop and parking lot storage, surface and underground tanks and storage in treatment units are the flow attenuation control alternatives. Wet weather quality control alternatives can be subdivided into two categories: primary devices and secondary devices. Primary devices take advantage of physical processes such as screening, settling and flotation. Secondary devices take advantage of biological processes and physical-chemical processes. These control devices are suitable for treating stormwater runoff as well as combined sewer overflows. However, the contact stabilization process is feasible only if the domestic wastewater facility is of an activated sludge type. The quantities of wet weather flows that can be treated by this process are limited by the amount of excess activated sludge available from the dry weather plant. At the present time, there are several installations throughout the country designed to evaluate the effectiveness of various primary and secondary devices. Based on these data, the representative performance of primary devices is assumed to be 40 percent BOD_5 removal efficiency and that of secondary devices to be 85 percent BOD_5 removal efficiency. No treatment is assumed to occur in storage. Hasan has synthesized available information regarding stormwater pollution control costs.[9] The results are shown in Table 1.

Table 1. Cost Functions for Wet Weather Control Devices[a,b,i]

Device	Control Alternative	Total Annual Cost: \$/yr $TC = wT^z$ or wS^z w	 z
Primary	Swirl Concentrator[c,d,e]	2,555.0	0.70
	Microstrainer[c,f]	9,179.8	0.76
	Dissolved Air Flotation[e]	10,198.1	0.84
	Sedimentation[e]	40,792.5	0.70
	Representative Primary Device Total Annual Cost = \$3,000 per mgd		
Secondary	Contact Stabilization[g]	24,480.4	0.85
	Physical-Chemical[e]	40,792.5	0.85
	Representative Secondary Device Total Annual Cost = \$15,000 per mgd		
Storage	High Density (15 per/ac)	51,000.0	1.00
	Low Density (5 per/ac)	10,200.0	1.00
	Parking Lot[h]	10,200.0	1.00
	Rooftop[h]	5,000.0	1.00
	Representative Annual Storage Cost[j] (\$ per ac-in) = \$122 $e^{0.16(PD)}$		

T = Wet Weather Treatment Rate in mgd; S = Storage Volume in mg

[a] ENR = 2200. Includes land costs, chlorination, sludge handling, engineering and contingencies.

[b] Sludge handling costs based on data from Battelle Northwest, 1974.[15]

[c] Field and Moffa, 1975.[10]

[d] Benjes, et al., 1975.[11]

[e] Lager and Smith, 1974.[7]

[f] Maher, 1974.[12]

[g] Agnew, et al., 1975.[13]

[h] Agnew, et al., 1975[13] and Wiswall and Robbins, 1975.[14]

[i] For T ≤ 100 mgd. No economies of scale beyond 100 mgd.

[j] PD = gross population density, persons per acre.

Optimal Mix of Storage and Treatment

The evaluation procedure for the nationwide assessment consisted of relatively detailed studies of five cities: Atlanta, Denver, Minneapolis, San Francisco, and Washington, DC. For each city, a single storm event for a selected catchment was simulated using the USEPA Storm Water Management Model (SWMM). Also, one year of hourly precipitation, runoff, and discharge rates were estimated using the HEC STORM model.[9] STORM estimates the total volume of storm water which is treated for a specified size of storage unit and treatment rate. Numerous combinations were tested for each of the five cities to derive storage/treatment isoquants as shown in Figure 1 for Atlanta. Given the storage/treatment isoquants and knowing the relative costs of storage and treatment, one can determine an optimal expansion path in terms of control costs versus percent BOD removal. The optimal expansion path is determined by comparing the costs of the various alternatives as shown in Figure 1, or

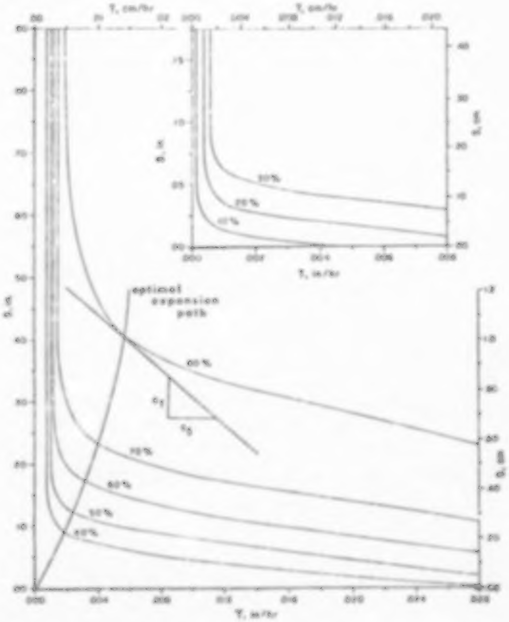

Figure 1. Storage/Treatment Isoquants for Various BOD Control Levels - Atlanta

$$\frac{c_T}{c_S} = MRS_{ST} \tag{1}$$

where c_T = unit cost of treatment,

c_S = unit cost of storage, and

MRS_{ST} = marginal rate of substitution of storage for treatment.

The above problem can be expressed in the more compact mathematical form shown below:

$$\text{minimize } Z = c_S(S) + c_T(T) \tag{2}$$

$$\text{subject to } f(R_1;S,T) = 0$$

$$R_1, S, T \geq 0$$

where Z = total annual control costs per acre,

$c_S(S)$ = storage costs,

$c_T(T)$ = treatment costs,

S = storage volume, inches,

T = treatment rate, inches per hour,

R_1 = percent pollutant control, and

$f(R_1;S,T)$ = production function relating the level of pollution control attainable with specified availabilities of storage (S) and treatment (T).

The storage/treatment isoquants are of the form:

$$T = T_1 + (T_2 - T_1)e^{-KS} \tag{3}$$

where T_1 = treatment rate at which isoquant becomes asymptotic to the ordinate, inches per hour,

T_2 = treatment rate at which isoquant intersects the abscissa, inches per hour, and

K = constant, inch^{-1}.

Substituting equation (3) into equation (2) and assuming linear costs, this constrained optimization problem can be solved by the method of Lagrange multipliers to yield the optimal mix of storage, S*, and treatment, T*, or

$$S^* = \max\left(\frac{1}{K}\ln\frac{c_T}{c_S}[K(T_2 - T_1)],\ 0\right) \tag{4}$$

and

$$T^* = T_1 + (T_2 - T_1)e^{-KS^*}. \tag{5}$$

Note that T* is expressed as a function of S*, so it is necessary to find S* first. Knowing S* and T*, the optimal solution is

$$Z^* = c_S S^* + c_T T^*. \tag{6}$$

The above optimization procedure was programmed to generate curves (e.g., Figure 2) showing percent pollutant removed versus total annual costs for primary and secondary treatment in conjunction with storage. The results indicated that the secondary treatment/storage curves could be used to estimate control costs over the entire range of interest. Note that, for wet weather control, marginal costs are increasing because of the disproportionately large sized control units needed to capture the less frequent larger runoff volumes. The curves shown in Figure 2 can be approximated by functions of the form:

$$Z = ke^{R_1 n} \tag{7}$$

where Z = total annual cost, dollars per acre per year,

k, n = parameters,

R_1 = percent pollutant removal, $0 \leq R_1 \leq \overline{R}_1$, and

$\overline{R}_1$ = maximum percent pollutant removal.

The five secondary cost curves and associated cost functions are shown on Figure 3. Note that the control costs per unit of runoff are much higher for San Francisco and Denver. This difference appears to be

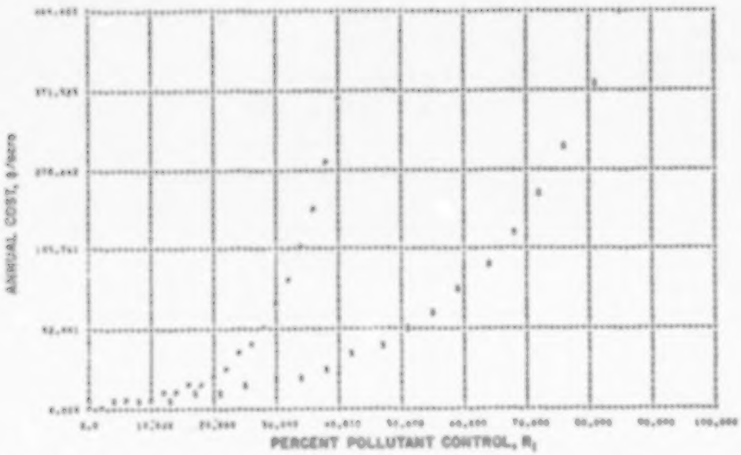

Figure 2. Control Costs for Primary and Secondary Units as a Function of Percent BOD Removal, Atlanta

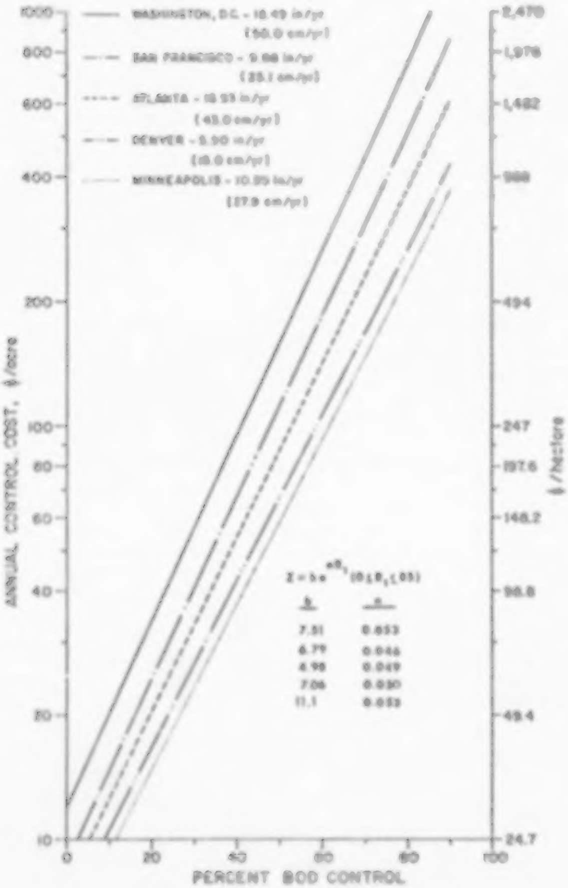

Figure 3. Control Cost for Secondary Units as a Function of Percent BOD Removal for the Five Regions (Preliminary Results, see Heaney, Huber, et al., 1976 for Final Results)

attributable to the different precipitation pattern in this part of the country. Thus, the five cities were aggregated into two major categories. The resulting preliminary estimating equations are shown below:

THIRTEEN WESTERN STATES

$$_{w}Z_{s} = (5.6 + 0.18AR)e^{0.05R_1} \qquad 0 \leq R_1 \leq 85 \qquad (8)$$

EASTERN STATES

$$_{e}Z_{s} = 1.8e^{(0.09AR + 0.05R_1)} \qquad 0 \leq R_1 \leq 85 \qquad (9)$$

where $_{e}Z_{s}$, $_{w}Z_{s}$ = annual cost using secondary control devices, dollars per acre, in the eastern (e) and western (w) US,

AR = annual runoff, inches per year, and

R_1 = level of BOD removal.

These equations are used for estimating the control costs for all of the urbanized areas in the US. One only needs to input the annual runoff, AR, and the desired level of control, R_1.

Runoff Prediction for Nationwide Assessment

Techniques for predicting runoff quantities vary from very simple methods of the Rational Method type to sophisticated models of the nature of SWMM. The technique used in STORM is relatively simple, relying on weighted average runoff coefficients and a simple loss function to predict hourly runoff volumes. Nonetheless, because of the nature of the continuous simulation involved, it is at a considerably higher level, and therefore more complex, than earlier, desk-top techniques. Due to the complexities and data requirements of STORM, it was not possible to run the model on all cities of the nationwide assessment, or even a majority. These considerations lead directly to the use of a simple runoff coefficient method in which runoff is merely a fraction of rainfall. STORM computes a runoff coefficient, CR, weighted between pervious and impervious areas by:

$$CR = 0.15\ (1 - I) + 0.90\ I \qquad (10)$$

$$= 0.15 + 0.75\ I$$

where I is fraction imperviousness and the coefficients 0.15 and 0.90 are the default values used in STORM for runoff coefficients from pervious and impervious areas, respectively. Note that the effect of demographic factors (e.g., land use, population density) is incorporated into the imperviousness. An equation developed by Stankowski[16] for New Jersey catchments was used to determine imperviousness as a function of population density, i.e.,

$$I = \frac{9.63}{100} PD^{0.573 - 0.039 \log_{10} PD} \tag{11}$$

where I = fraction imperviousness, and

PD = population density, persons per acre.

Thus, annual runoff, AR, from precipitation of P inches per year is

$$AR = CR(P). \tag{12}$$

Example

The generalized estimating equation will be applied to the Cincinnati, Ohio, urbanized area to illustrate the procedure. The requisite data are presented below[1]:

Demographic Data

1970 population = 1,110,000

developed area, A = 125,000 acres

population density, PD = 8.88 persons per acre.

Annual Runoff, AR

precipitation, P = 34 inches per year.

Using equation (12),

$$\begin{aligned} AR &= CR(P) \\ &= (0.15 + 0.75[0.0963(PD)^{0.573 - 0.039 \log_{10} PD}])P \\ AR &= 13.0 \text{ inches per year.} \end{aligned}$$

Control Costs for 60% BOD Control, R_1 = 60%

From equation (9)

$$_{e}Z_{s} = 1.8e^{(0.09AR + 0.05R_1)}$$

$$_{e}Z_{s} = \$116 \text{ per acre per year}$$

$$\text{Total annual costs} = {}_{e}Z_{s}(A) = \$116\ (125{,}000) = \$14{,}500{,}000 \text{ per year.}$$

Conclusions

A simple procedure for evaluating urban stormwater quality control costs is presented. This work is a condensation of the methodology used to develop a nationwide cost estimate for USEPA.[1] A detailed description of a more refined desk-top procedure for such evaluations will be released later this year.[5]

The reader is cautioned that the estimating equations (8 and 9) are preliminary. Final results will be presented in Heaney and Huber, et al., 1976.

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MODELING HYDROLOGIC-LAND USE INTERACTIONS IN FLORIDA

Philip P. Bedient
Asst. Professor
Envi. Sci. & Engr.
Rice University
Houston, Tex. 77001

Wayne C. Huber
Assoc. Professor
Envi. Eng. Sci.
Univ. of Florida
Gainesville, Fla. 32611

James P. Heaney
Assoc. Professor
Envi. Eng. Sci.
Univ. of Florida
Gainesville, Fla. 32611

Summary

A technique is developed to describe and quantify various hydrologic-land use interactions within a Florida river basin. Surface runoff quantity and quality are estimated as a function of land use and drainage patterns at several levels of resolution including the river basin, tributary watersheds, lake basins, and marsh areas. A hydrologic-land use model based on a daily water balance is applied to each soil-land use complex in the watershed to estimate soil storage and total runoff. The overall basin response seems to be more sensitive to the land drainage pattern than to the condition of the narrow river flood plain.

Potential nutrient loading rates are calculated using measured concentrations of total P and predicted runoff volumes. The drainage density index correlates with observed concentrations and loading rates for the tributary watersheds. The detention time parameter for various hydrologic components in the basin indicates the potential for control of runoff quantity and quality through on-site storage in marsh, pond, and lake areas. Excessive drainage activities have led to higher nutrient loads and decreased detention times in the river basin.

Introduction

Traditional approaches to watershed analysis have placed little emphasis on linkage mechanisms which relate land use and drainage conditions to resulting hydrologic and water quality responses in a watershed. Measured changes in land use and drainage patterns provide a useful starting point for estimating the impact of alternative future levels of development. Environmental responses which can be measured or predicted include the volume of surface runoff and streamflow, and associated pollutant concentrations or loadings which stimulate aquatic plant growth.

The main objective of this research is to describe and quantify various hydrologic-land use interactions which occur within a river basin, in order to estimate the historical, present, and projected environmental responses in the basin. This requires that a technique be devised to characterize surface runoff quantity and quality as a function of land use and drainage patterns. Influences of soil storage, vegetative cover, drainage intensity, land use, topography, and climate are directly considered in the formulation.

It is important to consider these interactions at several levels of resolution or detail in order to better understand the overall response of the watershed. Various levels which are investigated include the river basin, lateral tributary systems, lake units, and marsh drainage areas. Analyzing the response of these different components allows quantification of storage and transport mechanisms through the system.

Description of the Study Area

The Kissimmee River Basin, located in central Florida, is undergoing pressure for both agricultural and urban expansion, while vast, undeveloped marsh areas in the basin provide a valuable environmental resource. This basin provides a convenient study area because of the quantifiable land use changes and water quality responses which have been observed over the recent past.

The original river began near the Orlando area and passed through a series of shallow lakes before emerging south of Lake Kissimmee as a meandering river. It then flowed south to Lake Okeechobee through a relatively narrow marsh flood plain (Figure 1). Presently, the upper portion of the basin consists of a chain of large lakes undergoing rapid urbanization from the surrounding Orlando area. The lower basin is undergoing transition from its undeveloped state as a marsh/swamp system to a regime dominated by improved pasture with lateral drainage canals. In addition to the land use changes, an extensive flood control project has been implemented by the Corps of Engineers with control structures at the outlet of the lakes and along the channelized main river.

Water quality degradation in the form of high nutrient loading in one of the upper lakes and along the river channel has been increasing over the last two decades. There is concern for protecting water quality since the Kissimmee River is the main inflow to Lake Okeechobee, which provides water supply to all of south Florida and the Everglades. Objections have been raised by ecologists and conservation groups over the destruction of a unique, natural meandering river and its rich marshes, the decline of fish and waterfowl resources, and the effect of degraded water quality on the eutrophication of Lake Okeechobee.[1] During the past two years, intensive studies by several groups have been underway to examine the environmental resource problems in Lake Okeechobee and the Kissimmee River Basin. The development and application of environmental simulation models along with pertinent results are discussed in the following sections.

Land Use Analysis

Land use in the Kissimmee River Basin has undergone rapid and significant changes in the last 15 years. Past activities in the upper part of the basin (1958) were dominated by urban interests, especially around the Orlando area, and agricultural interests involved in citrus on the eastern ridge, small amounts of improved pasture throughout the remainder of the basin. The dominant undeveloped category was freshwater marsh and swamp around the large lakes and adjacent to the Kissimmee flood plain. The 1972 land use patterns show about 40 percent of the land which was formerly unimproved pasture has been improved through diking or drainage procedures. Large areas of marsh and swamp have been converted to improved or unimproved pasture. In addition, urban expansion is evident south of Orlando, around lake borders, and in the Disney World area of western Orange County.

Future patterns of land use in the Kissimmee River Basin have been projected using estimates of the Soil Conservation Service (SCS) and the U.S. Department of Agriculture in conjunction with a linear programming model developed in the study. The results of this analysis are projections, to the years 1980, 2000 and 2020, of what land use could be.

A more complete description of the land use methodology is available, and the results of the analysis serve as direct input to the hydrologic-land use model discussed below.[2] The observed shifts in land use and drainage practices have already created a series of effects which have begun to jeopardize the region's ability to cope with increasing runoff volumes and degraded water quality from waste loads.

Hydrologic-Land Use Interactions

Introduction

Relatively little research has been done on problems associated with watersheds dominated by marsh and lake storage, extremely flat slopes, and long-term seasonal rainfall and flooding. These are termed depressional watersheds, and are most commonly found along the Coastal Plain of the southeastern United States. South Florida watersheds including the Kissimmee-Everglades region fall into this category.

Because the hydrologic response of the drainage basin is the controlling link for land use and water quality considerations, a hydrologic-land use model (HLAND) has been developed which directly incorporates land use changes and drainage practices. The model is based on the daily water balance technique of Thornthwaite and the Soil Conservation Service runoff curve number method applied to each soil-land use type in each subwatershed.[3,4] The technique places primary emphasis on soil storage and potential evapotranspiration (PE) dynamics to determine surface and subsurface runoff volumes on a daily basis. The approach is ideally suited for modeling depressional watersheds.

Hydrologic-Land Use Model Description

The climatic water balance was first developed in an effort to characterize the moisture condition of an area based on a balance between precipitation (P) which adds moisture to soil storage and evapotranspiration (ET) which removes it. Knowledge of the relationship between P and ET provides information on periods of moisture surplus (S) and moisture deficit (D), which in turn provides data on irrigation requirements, surface runoff, groundwater recharge, and soil moisture storage.

The various terms and relationships involved in the water balance are shown in Figure 2. The budget can be run on a monthly, weekly, or daily basis depending on the desired accuracy. Measured values of precipitation (P) and calculated potential evapotranspiration (PE), which can be determined for a region by any one of the available techniques, provide the initial value of excess precipitation (P-PE).[5] If this value is positive, then soil moisture storage (ST) is increased up to the maximum level (SM), and actual evapotranspiration (AE) equals PE. A water surplus (S) is generated above the ground surface if (P-PE) exceeds (SM-ST) for a given time increment. For this condition,

$$S = (P-PE) - (SM-ST) \tag{1}$$

If the value of (P-PE) is negative, then a loss occurs from soil moisture storage. The loss is not linear, because as the soil dries, plants are less able to remove water via evapotranspiration due to capillary forces. Thornthwaite assumes that the actual amount of removal is proportional to the level of soil moisture content. This condition can be expressed by an exponential relation of the form

$$ST = (SM)\, e^{-(DWL \times AWL)} \tag{2}$$

where DWL = depletion coefficient, and
AWL = accumulated water loss.

Resulting curves for various levels of SM are plotted in Figure 2. Thus, for the case of curve A, if the accumulated water loss is 50 mm, the resulting soil moisture retained (ST) is 62 mm. Because ST is less than SM, the AE term is no longer equal to PE for the case of negative (P-PE). Instead,

$$AE = P + |\Delta ST| \tag{3}$$

where

$|\Delta ST|$ = available moisture which can be removed from the soil, over one time step.

The difference between PE and AE is termed the water deficit (D).

The water balance technique is a powerful predictive tool for areas undergoing land use and vegetative changes, increased drainage, and/or urbanization. Drainage of land generally causes a reduction in soil storage, an increase in surface runoff, and a decrease in groundwater levels, all of which can be quantified using the water balance. Increases in irrigation requirements can also be predicted based on increasing moisture deficits from drainage.

The HLAND Model computerizes the Thornthwaite water balance for calculation of daily runoff using daily rainfall values from each soil-land use type in the study area. Several additional components have been incorporated to better represent the hydrologic response. A more detailed description of the model and input data is available.[6]

The SCS runoff curve number CN(J,K) for land use J and soil group K is used to estimate maximum soil moisture storage SM(J,K) by the equation

$$SM(J,K) = \frac{1000}{CN(J,K)} - 10 \tag{4}$$

Typical values of SM in the Kissimmee River Basin range from 2 inches for drained improved pasture to 23 inches for some of the marsh areas.

Predicted surplus volumes do not become runoff instantaneously. Rather, overland flow is delayed by specifying that a fraction CDET(J,K) of the available surplus will remain on the land per day. These detention constants are estimates derived from Thornthwaite and Mather and the SCS, and vary from 0.60 for drained improved pasture to 0.90 for marshes and swamps.[7,4] These constants allow the surplus to become runoff at an exponential rate, or in direct proportion to the amount available. Average detention time in days can be derived from the detention coefficients for each soil-land use type.

Base flow contributions as a function of soil moisture storage have been specifically determined for the Kissimmee River Basin.[8] The relation was obtained through the technique of hydrograph separation for 15 years of streamflow data for the Kissimmee River. Base flow is incorporated into HLAND by fitting an equation to Langbein's relation, and partitioning the subsurface flows to each soil-land use complex in each planning unit. In this way, base flow is calculated as a function of soil moisture storage on a given day, and then subtracted from soil storage at the end of the day If another type of base flow relation is preferred, it can easily be incorporated into the model.

Flood Routing and Model Calibration

Extensive and costly flooding occurred under natural conditions in the Kissimmee River Basin due to prolonged seasonal rainfall, inadequate secondary drainage, and limited outlet capacity. Tropical hurricanes, which usually occur during the rainy season, also served to intensify the problems. The existing flood control project was implemented in the 1960's and provided for channelization and control structures on the Kissimmee River and below the large upper basin lakes.

A comparison of flood hydrographs with and without the flood control project indicates significant differences regarding both the shape and magnitude of the response. The 1969 hydrograph is characteristic of a developed drainage system with higher peak flows, shorter lag times, and shorter recession times; compared to flood events prior to channelization and upland drainage.

The model HLAND was verified for the Kissimmee River Basin using both 1958 and 1972 land use conditions and a series of historical daily rainfall patterns over the basin. HLAND calculates the contribution of total runoff to the river, and a flood routing procedure is used to simulate either the original meandering river or the present channelized regime. In this way, it is possible to determine the relative effects of river channelization vs. upland tributary drainage on observed outflow hydrographs.

While sophisticated flood routing methods are available, the linear Muskingum method is ideally suited for modeling the daily response in depressional watersheds where long-term seasonal effects are of primary concern.[9] Storage and travel time parameters are adjusted to the original river or channelized regime.

A series of calibration years, 1965-1970, was selected based on the availability of data and the fact that this sequence includes both drought and extreme flood conditions, which provides a good test of the accuracy of the model. A comparison of measured and predicted streamflows for 1972 land use conditions is depicted in Figure 3 at the gaging station near Lake Okeechobee (S65-E). It can be seen that the model provides a generally accurate representation of the basin response during conditions of floods (1969-1970), droughts (1965-1967), and average flows (1968).

Based on calibration runs using 1958 land use and the original flood plain, the basin response seems to be much more sensitive to the land drainage characteristics than to the condition of the narrow river flood plain. Overall travel times in the system were slower under the 1958 regime because upland marsh and slough detention provided additional storage capacity during the wet season. The present regime induces excess water into drainage canals at a faster rate, and HLAND results indicate increasing percentages of surface runoff compared to subsurface flows as upland drainage activity increases. Thus, lateral subwatersheds dominated by drainage canals tend to produce more surface runoff than those in a more natural drainage condition, while subsurface contributions are less under drained conditions due to decreased soil moisture levels.

Water Quality Considerations

Monitoring Program

Water quality data have been collected in the Kissimmee River for the past several years, and in tributary inflows for the 1973-74 period. The monitoring program was begun by the U. S. Geological Survey, and has been continued and expanded by the Central and South Florida Flood Control District (FCD).[2]

An analysis of available water quality data from the FCD indicates that total and inorganic phosphorus levels are the most responsive parameters compared to nitrogen variation. Phosphorus tends to adsorb to soil particles and is readily available for surface transport via runoff and erosion.

Samples were taken monthly for one year for the lower river stations and the major upper lakes in the basin. A plot of average wet season total P concentrations along the extent of the basin indicates a rapid decline through the lake system and a further increase along the channelized portion of the river (Figure 4). The high levels in the upper lakes are primarily due to nutrient loading from treated sewage effluent, and it appears that the lakes are serving as nutrient sinks at the present time.

The water entering the channelized Kissimmee River is of fairly good quality, but concentrations increase rapidly below structure S65-C. Detailed analyses of tributary inflow quality by the FCD indicate progressively higher P concentrations, especially south of S65-C, which correlates with the observed trend in the river. There is a need, then, to explain the observed distribution of surface runoff and nutrient loading in the basin as a function of land use and drainage activities.

Drainage Density and Pollutant Loading

While the hydrologic model estimates source areas which contribute runoff volumes, non-point sources of nutrients are primarily a function of land use, with agricultural lands contributing relatively high loads due to fertilization of cattle density. Loehr has surveyed the available literature to determine relative loading rates from various land uses.[10] Potential nutrient loading rates can be calculated for each subwatershed in the basin using measured concentrations of total phosphorus and predicted runoff volumes from HLAND. Higher loading tends to be associated with higher runoff rates in areas of intense drainage.

Detailed analyses of land use and drainage patterns along the lower river system indicate the importance of the drainage density index, measured in miles of drainage network per square mile of land area. Drainage density provides a useful general indicator of land use intensity, runoff volumes, and nutrient concentration associated with the various tributaries in the Kissimmee River Basin.[11]

When drainage density measurements are compared with measured inflow concentrations of average total P during the wet season, positive correlations are obtained. Converting to phosphorus loading rates as a function of tributary drainage density yields the significant relationship in Figure 5. Although only a limited number of data points are available for the lower basin, the results compare favorably with values reported in the literature for agricultural loading rates.[12] It is reasonable to expect this result since drainage density is inversely related to the average length of overland flow, an indicator of potential runoff and pollutant transport.

Storage-Treatment Concepts

Characteristics of hydrologic and nutrient cycles can be placed into the general framework of reservoir storage and control. Various hydrologic components in a river basin system are distinguished by a set of specific inflows, outflows, storages, and losses which contribute to the overall response. The detention time parameter, $\bar{T}$, defined as the ratio of storage volume to outflow rate, can be used to characterize various components of the hydrologic system, e. g., soil, marsh, pasture, lake, subwatershed or river.

Detention time also plays a key role in nutrient cycling as it relates to treatment rates for runoff on the land, in the soil, and in lakes or streams. In general, the longer the detention time, the greater the potential for nutrient uptake and/or deposition of sediments. Thus, water quality control through the system can be characterized by the length of time available for physical, biological and chemical uptake mechanisms.

Calculated detention times from the HLAND results average about 130 days in the soil system, and range from 1.5 to 9.5 days for surface runoff from various land uses. Subwatersheds characterized by intensive drainage activity tend to have lower average detention times, 2.2 days compared to 4.5 days for naturally drained areas.

The flood routing technique in the river channel uses a travel time or detention time of 3.5 days compared to a possible upper limit of 9.0 days for the original flood plain condition. These relatively short detention times result in a low potential for nutrient uptake in the river or flood plain alone.

Since nutrient uptake requires long detention times, the greatest potential would occur in lakes and marsh storage areas, which also provide a measure of flood storage capacity. Average detention times in Lake

Tohopekaliga south of Orlando varies from 4.0 to 6.0 months in wet and dry seasons, and can drop as low as 1.0 month during extreme floods. Although nutrient loading is excessive to the lake, long detention times allow for up to 85% uptake by the time the water leaves the lake (Figure 4). If future developments around the lake basin should cause a reduction in detention time from 4.0 to 2.0 months, then uptake potential could drop to 67%.

The detailed study of a marsh area above S65-D reveals a definite potential for flood attenuation and nutrient uptake. Results from a marsh routing model indicate that detention times from 3.0 to 5.0 days provide from 30 to 55% uptake of total P, based also on field data. Thus, marsh areas provide a significant potential as long as routed runoff volumes through them do not reduce detention times below 3.0 days. These concepts are presently being tested in the basin.

In general, marsh and lake detention times are comparable on a per acre basis to the soil system. However, both the surface runoff and river system are distinguished by considerably smaller values of T, around 5.0 days for the entire river. Thus, the potential for control of runoff quantity and quality in the basin exists through on-site storage in marsh, pond, and lake areas. Excessive drainage activities have led to higher nutrient loads and decreased detention times.

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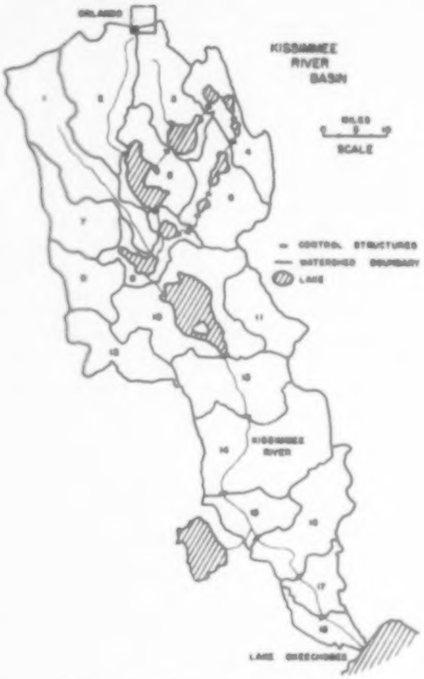
ORLANDO
KISSIMMEE RIVER BASIN
MILES
SCALE
CONTROL STRUCTURES
WATERSHED BOUNDARY
LAKE
KISSIMMEE RIVER
LAKE OKEECHOBEE

Figure 1. Location Map

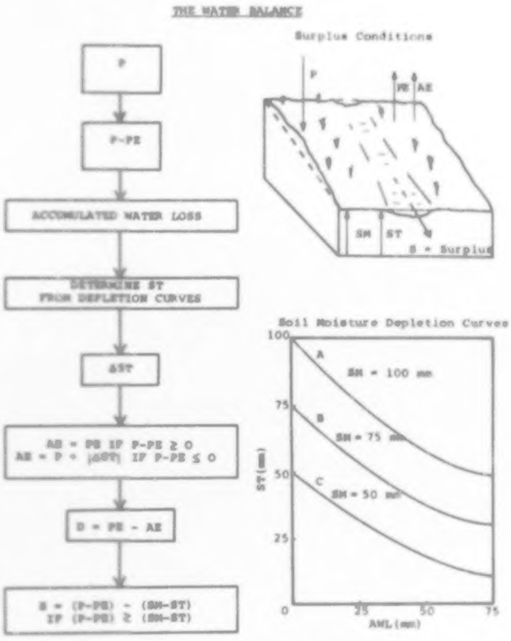
THE WATER BALANCE
P
P-PE
ACCUMULATED WATER LOSS
DETERMINE ST FROM DEPLETION CURVES
ΔST
AE = PE IF P-PE ≥ 0
AE = P + |ΔST| IF P-PE ≤ 0
D = PE - AE
S = (P-PE) - (SM-ST) IF (P-PE) ≥ (SM-ST)
Surplus Conditions
P
PE
AE
SM
ST
S = Surplus
Soil Moisture Depletion Curves
A
SM = 100 mm
B
SM = 75 mm
C
SM = 50 mm
ST (mm)
AWL (mm)
0
25
50
75
100

Figure 2. The Water Balance

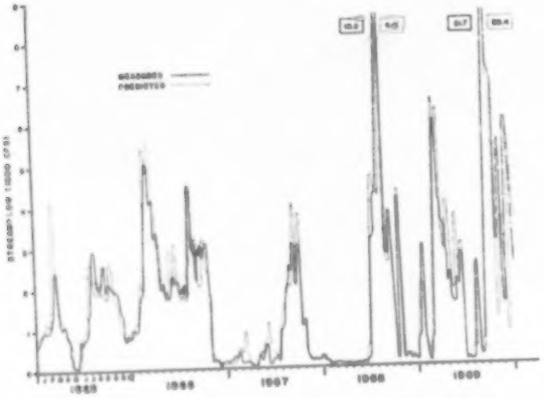

Figure 3. Calibration Curves in the Kissimmee River Basin

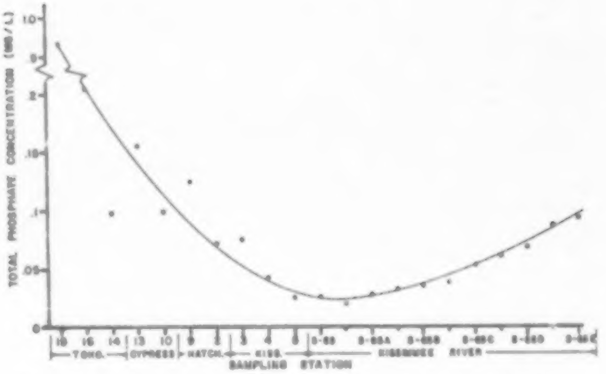

Figure 4. Observed Phosphorus Concentrations in the Kissimmee River Basin

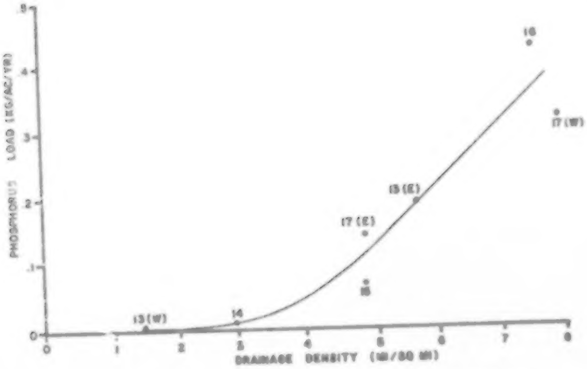

Figure 5. Phosphorus Load vs. Drainage Density

MODELING URBAN RUNOFF FROM A PLANNED COMMUNITY

Elvidio V. Diniz, Espey-Huston and Associates, Austin, TX
Don E. Holloway, Espey-Huston and Associates, Houston, TX
William G. Characklis, Rice University, Houston, TX

Summary

A management strategy for utilization of water resources in the planned community of The Woodlands, near Houston, Texas, is being developed by modification and application of the EPA Storm Water Management Model (SWMM). Selected sites on Panther Branch, which flows through The Woodlands, and on Hunting Bayou, a completely developed watershed within the city limits of Houston, Texas were modeled for testing and verification of the modifications to the SWMM.

The capacity of the SWMM to model urban runoff quantity has been improved to include the "natural" drainage concepts of The Woodlands and the infiltration computation model in the SWMM is now capable of operating with a rainfall record which includes periods of zero rainfall. Three new subroutines have been written to operate in conjunction with the SWMM. The three subroutines generate normalized area-discharge curves for natural sections, model baseflow conditions, and model the operation of porous pavements, respectively. Verification of the SWMM with regard to suspended solids and BOD_5 was attempted and modifications to predict COD, Kjeldahl nitrogen, nitrates and phosphates were performed.

Scope of Study

Increased runoff rates and increased pollutant loads are two of the major effects of urbanization on the hydrologic regime of a previously undeveloped watershed. The increase in impermeable areas due to urbanization results in high velocity surface flows which tend to increase the potential for capture of pollutants by the storm water and reduce natural infiltration processes.

The planned new community of The Woodlands is designed to minimize the detrimental effects of urbanization upon the runoff characteristics of the watershed in which it is located. Several extensive changes to the U.S. Environmental Protection Agency Storm Water Management Model (SWMM) had to be performed to allow modeling of storm water runoff in The Woodlands by use of the SWMM. The necessary changes to the SWMM include modified computations for infiltration volumes and pollutographs and three new subroutines to develop normalized area-discharge curves for natural channel sections, to model baseflow conditions, and to model runoff from porous pavements. This paper discusses the changes that were performed to the SWMM, the new subroutines that were developed, and the concurrent modeling effort in The Woodlands. An urban Houston watershed, Hunting Bayou, was also modeled because its drainage characteristics are similar to those of The Woodlands.

The Woodlands Study Area

The Woodlands is a planned urban community being developed approximately 28 miles north of Houston, Texas in a heavily forested 17,800 acre tract in Montgomery County. A total of 33,000 dwelling units with a projected population of 112,000 is programmed at project completion in 1992. A concern for nature and convenience for people are two of the major criteria used in the development of the General Plan for The Woodlands, consequently, all development in The Woodlands is based on a comprehensive ecological inventory conducted from 1971 to 1973[1]. Approximately 33 percent of the total area, including all flood-prone land, is planned for open space uses. Some of the open space will be retained in its original state to provide wildlife habitat, while other areas will be maintained for park and similar recreational uses.

The Woodlands site is located in the Spring Creek Watershed. Panther Branch, an intermittent tributary to Spring Creek, is the major drainage channel as shown in Figure 1. Drainage channels tributary to Panther Branch and Spring Creek are characterized by broad and shallow swales having very mild slopes.

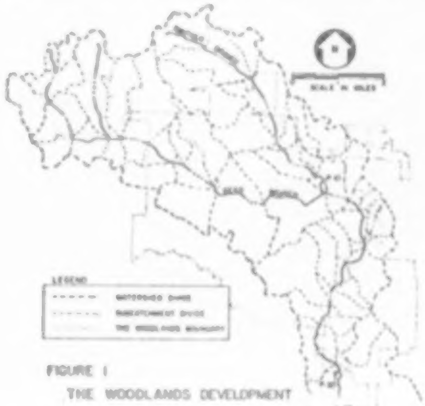

FIGURE 1
THE WOODLANDS DEVELOPMENT

A detailed soil survey by the U.S. Department of Agriculture Soil Conservation Service and the Texas Agricultural Experiment Station determined that the soils in The Woodlands site are highly leached, acid in reaction, sandy to loamy in texture and low in organic content. The vegetation is typical for a mixed woodlands of the Southern Piney Forest characterized by loblolly and short-leaf pines in association with hardwood species, including oak, sweet gum, hickory and magnolia[1]. The dense vegetation, sandy soils and mild slopes result in high retention and infiltration losses from rainfall.

The design of all drainage channels in The Woodlands is based on the premise that typically narrow and deep drainage ditches are undesirable. Therefore, the existing drainage channels are utilized to the fullest extent possible and any new channels are constructed as wide, shallow swales and lined with native vegetation to emulate the existing channels. Storm sewers and drains are used in high density and activity areas to conduct the excess runoff to the nearest drainage channel with sufficient capacity to safely carry the flow. To minimize increases in runoff volumes and peaks, retention ponds are utilized whenever practical.

The net effect of this "natural" drainage system is an increase in infiltration and storage capacity in the channels, thereby reducing the impact of urbanization upon the runoff regime.

Data Sampling and Sources

There are two stream stage recorders located on

Panther Branch: Panther Branch near Conroe (P-10) and Panther Branch near Spring (P-30) as shown in Figure 1. Station P-10, located below the confluence of Panther and Bear Branches, measures runoff from 25.1 sq mi of undeveloped forest land. Station P-30 has a drainage area of 33.8 sq mi with the developing areas of The Woodlands (Phase I) immediately upstream.

The Hunting Bayou study area is located northeast of downtown Houston and within the metropolitan confines of the city. As seen in Figure 2, there are two gaging stations: Hunting Bayou at Cavalcade Street (H-10) and Hunting Bayou at Falls Street (H-20). The drainage areas of Stations H-10 and H-20 are 1.03 and 3.08 sq mi, respectively. Land use is primarily residential with some commercial and industrial areas. There are very few storm sewers and the major portion of the drainage system is made up of grass-lined swales comparable to those of The Woodlands.

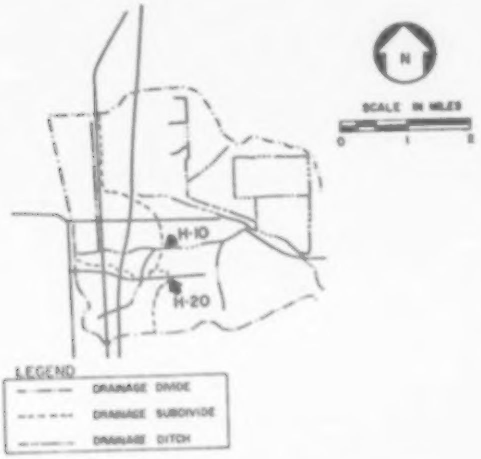

FIGURE 2--THE HUNTING BAYOU WATERSHED

During storm events, streamflow quality sampling was conducted in conjunction with flow gaging. The samples were analyzed for a large number of parameters including suspended solids, COD, nitrates, phosphates and Kjeldahl nitrogen. Reconstitution of the observed hydrographs and pollutographs to calibrate the SWMM were attempted in the modeling effort.

Modifications to the SWMM

The SWMM was originally developed to model the hydrologic effects of older urban areas where an artificial drainage system was imposed upon, and in most cases entirely replaced, the original drainage system. In the application of SWMM to The Woodlands, several deficiencies in the model were encountered. The major modifications are discussed in the following sections.

Modification to Infiltration Volume Computation

Infiltration rates are computed in the RUNOFF Block of the SWMM by means of Horton's Equation defined as follows:

$$f_c = (f_i - f_o)\, e^{-kt^*} + f_o$$

where:	f_c	infiltration rate at time t^*
	f_i	initial infiltration rate
	f_o	final infiltration rate
	k	decay coefficient
	t^*	time from start of rainfall to the midpoint of the time interval Δt; or $t^* = t + 0.5\,\Delta t$

The RUNOFF Block of the SWMM was structured such that Horton's time dependant infiltration rate decay equation would become operative from the start of modeling time. Consequently, if the time of start of rainfall did not coincide with the start of modeling time, the infiltration rate would have decayed to a lower rate by the time rainfall had begun. This may be one reason why early investigators determined that the starting infiltration rate was not a significantly sensitive parameter[2]. A second problem with the computation of infiltration volume resulted from the input of two or more high intensity rainfall events separated by time periods of zero or low intensity rainfall that was not capable of satisfying the infiltration rate. The infiltration rate would decay without regard to the availability of rainfall for infiltration. Modeling runoff under these conditions was difficult and consequently the infiltration computation method in the SWMM was modified.

The new computation scheme uses an integral form of Horton's Equation and a time parameter to monitor the progress of infiltration only. The integral of Horton's Equation is:

$$M = f_o t + \frac{(f_i - f_o)}{k}(1 - e^{-kt})$$

where:	M	accumulated infiltration volume in inches at the end of time t

The other variables are as defined previously

During each time interval (Δt), the volume of water capable of infiltrating ($M_{t+\Delta t} - M_t$) is calculated and compared to the total volume of water available for infiltration determined as

$$D_t = S_t + R_t\,\Delta t$$

where:	D_t	water volume after rainfall during time interval Δt
	S_t	water volume remaining from the previous Δt
	R_t	intensity of rainfall during Δt

When the available volume is greater than the infiltration volume, the excess is calculated as the volume of water available for runoff. The results are comparable to those previously computed by the SWMM.

If the infiltration volume is greater than the available volume, the time increment, $\Delta t^* < \Delta t$, is computed such that the infiltration volume is equal to the available volume:

$$M_{t+\Delta t^*} - M_t = D_1$$

where:	$M_{t+\Delta t^*}$	volume of infiltration at time $t+\Delta t^*$
	M_t	volume of infiltration at time t
	D_1	volume of water available for infiltration

and no runoff is generated for that Δt.

The infiltration rate at time $(t + \Delta t^*)$ then becomes the starting infiltration rate for the next computational time interval beginning at time $(t + \Delta t)$. Therefore, the elapsed time for infiltration rate decay by Horton's Equation will not necessarily coincide with the elapsed runoff computation time.

Subroutine NATSEC

In the TRANSPORT Block of the SWMM, normalized area-discharge curves are required for flow routing. Thirteen uniform channel shapes (circular, rectangular, trapezoidal, etc.) have their respective curves preprogrammed through Block Data, but those for natural sections have to be independently computed and input to the model. Because of the large volume of work required in preparing these curves for a "natural" drainage system, Subroutine NATSEC was written and incorporated into the SWMM. This subroutine generates normalized area-discharge curves for irregularly shaped cross sections and for cross sections with varying values of Manning's roughness coefficient, n. The cross section is input to the subroutine by means of a two-dimensional linear coordinate system. Three Manning's n values, one for each overbank and one for the channel, may also be used. Depth increments for equal increments of area are calculated by an iterative process.

When the depth of flow is below bank elevations, a single application of Manning's equation is sufficient. If the channel capacity is exceeded, the flows in each overbank as well as flows in the channel are computed by independent applications of Manning's equation to each flow area. The total discharge is equated to the sum of the individual discharges.

The output from subroutine NATSEC is a tabular version of the normalized area-discharge curves for natural channels and is comparable to the other area-discharge curves in Block Data of the SWMM.

Subroutine BASFLO

The SWMM computational scheme considers all infiltration volume as permanently removed from the runoff volume. The volume of rainfall that soaks into vegetation debris and surface soils and which drains out at a very delayed rate is not accounted for because in most urban areas this interflow volume is negligible. But, again, in the "natural" drainage system of The Woodlands, interflow does become a significant factor. In vegetated areas, the volume of infiltration as computed in the SWMM includes evapotranspiration losses and losses to groundwater. Interception losses may be accounted for in either the infiltration or surface depression storage.

The portion of the hydrograph beyond the point of inflection (where $dQ/dt \to \infty$) is generally considered as depletion of runoff volume stored in the drainage system or watershed. As for most depletions in nature, the rate of depletion approximates an exponential decay and is often referred to as baseflow recessions[3] of the form:

$$Q_{t+\Delta t} = Q_t \, e^{-k\Delta t}$$

where:		
	$Q_{t+\Delta t}$	flow at end of time interval Δt
	Q_t	flow at start of time interval Δt
	k	recession coefficient

The recession coefficients and their associated flow ranges are user-supplied to Subroutine BASFLO. One theory of varying recession coefficients for a single hydrograph is the concept of drainage of different storage units in the hydrologic system[4]. In The Woodlands, both stations P-10 and P-30 exhibit 2 recession ranges. The recession coefficients (determined from observed hydrographs) are plotted against the flow at start of recession and the corresponding regression equations are derived. The coefficients of the regression equations are input to Subroutine BASFLO. All flow rates beyond the point of inflection are determined by consecutive applications of the recession coefficient regression equations and the baseflow recession equations.

Subroutine BASFLO also provides for inclusion of the groundwater component of runoff. The groundwater flow rate may be input as a constant, linearly varying, or logarithmic function. All computed groundwater flow rates are added to the runoff hydrograph with respect to time resulting in a corresponding upward shift in the runoff hydrograph.

The baseflow rates are substituted into the runoff hydrograph prior to addition of groundwater flow rates. The specific water quality loading rates are applied to the new flow rates and the corresponding pollutographs are computed.

Subroutine PORPAV

The Woodlands Development Corporation has envisaged an extensive use of porous pavements in the place of conventional impermeable pavements. Subroutine PORPAV was developed to model the effects of porous pavements on the runoff volume and peak flows because the SWMM did not have this capability.

The modeling scheme consists of delineating the porous pavement and the subgrade as two hydraulically connected control volumes for which the inflow and outflow conditions are established by the equation for continuity or conservation of mass:

$$\frac{ds}{dt} = I - O$$

where:		
	$\frac{ds}{dt}$	change in storage during time interval dt
	I	time average inflow
	O	time average outflow

Inflow to the porous pavement area is determined as the sum of direct rainfall onto the pavement and the overland flow hydrograph as computed by Izzard's method[5].

The outflow is the sum of vertical seepage losses, horizontal seepage losses, surface runoff when the porous pavement storage capacity is exceeded, and evaporation losses. Vertical seepage losses are computed by the variable head permeability equation. A modified Darcy Equation is used to model the horizontal seepage losses and Manning's Equation is used to establish the surface runoff rate. The instantaneous evaporation loss rate is computed from a time-lagged sine curve approximation of diurnal evaporation loss rates.

Unfortunately, no data on existing porous pavements are available. Therefore, all testing of Subroutine PORPAV has been done on a hypothetical area.

Storm Water Quality Modeling

A thorough analysis of the available water quality data from The Woodlands was conducted in an attempt to define a methodology to predict runoff quality, specifically nitrates, phosphates, Kjeldahl nitrogen, and

COD. The present version of the SWMM considers these as percentages of the dust and dirt volume. Recognizing that in The Woodlands the dust and dirt generation rates are not typical of other urban areas, relationships between quantity and quality of flow were sought. Plots of cumulative pounds of pollutant versus cumulative volume of flow indicate a strong relationship as shown in Figure 3.A for COD. In some cases, if availability of the pollutant is exceeded, the upper portion of the straight line will curve upwards indicating that the rate of pollutant loading is decreasing with increasing flow. Also, it was determined that total pollutant loading in units of pounds per acre is a function of total inches of runoff as shown in Figure 3.B for COD. The slopes of the straight lines tend to increase with urbanization, indicating an increase of pollutant loading for the same volume of runoff. The relative magnitude of the urbanization effects may be determined by the increase in slope.

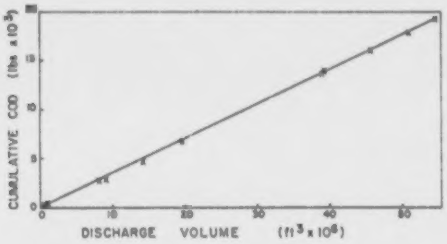

FIGURE 3.A--DOUBLE MASS ANALYSES
FOR THE STORM OF 12/05/74 AT GAGE P-30

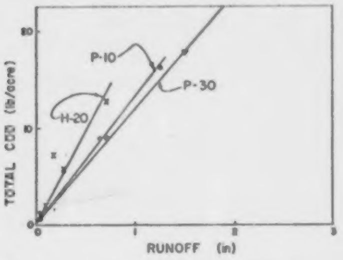

FIGURE 3.B--TOTAL POLLUTANT LOADING RATES

The pollutant loading relationship may be used to determine total pollutant mass and the cumulative pollutant mass relationship can provide a flow dependent mass transport rate. A combination of the two functions can be used to develop a pollutograph.

This methodology to determine quality of runoff is unrelated to the dust and dirt accumulation approach as used in the SWMM. Consequently, the quality of runoff computations in the SWMM would have to be completely rewritten to incorporate the new methodology. A simpler modification involves the input of user supplied pollutant loading rates. Initial modeling attempts using this approach are now being conducted.

Application of SWMM to The Woodlands and Hunting Bayou

The 33.8 sq mi of drainage area upstream of Station P-30 was divided into 57 subcatchments with an average size of 380 acres. Physical parameters were determined from topographic maps obtained from the U.S. Geological Survey and The Woodlands Development Corporation. Certain parameters such as width of subcatchment and retention depths cannot be directly determined for natural watersheds. Therefore, these parameters can be adjusted within reason so that a good fit exists between observed and computed hydrographs. Width of subcatchment values were first estimated using the method described in the SWMM User's Manual. These values had to be reduced by approximately 40 percent because overland flow will not occur as sheet flow over the entire subcatchment.

The parameters for infiltration modeling at Stations P-10 and P-30 are listed in Table 1. Table 2 lists the observed and computed peak flows and volumes and Figures 4 and 5 compare the observed and computed hydrographs and suspended solids pollutographs for the storm of 12/05/74 at Stations P-10 and P-30, respectively. The SWMM predicts suspended solids transport very well at the P-10 gage, but the prediction at the P-30 gage is not as successful. One reason may be the transient state of construction and development in the drainage area between the two gages. Accounting for all construction areas and their erodibility prior to the storm event being modeled proved to be difficult. Consequently, it is presumed that several construction areas where the natural ground had been disturbed and stripped of the protective vegetative cover contributed more suspended solids than the SWMM could predict from the available input data.

TABLE 1 -- INFILTRATION PARAMETERS FOR
PANTHER BRANCH WATERSHED

STORM DATE	STATION	INFILTRATION RATES Initial in/hr	Final in/hr	Decay /sec
10/28/74	P-10	3.5	0.01	.0005
	P-30	3.5	0.01	.0005
11/10/74	P-10	0.3	0.01	.00115
	P-30	0.3	0.01	.00115
11/24/74	P-10	2.0	0.01	.00115
	P-30	2.0	0.01	.00115
12/05/74	P-10	0.5	0.01	.00115
	P-30	0.5	0.01	.00115
12/10/74	P-10	0.2	0.01	.00115
	P-30	0.2	0.01	.00115

TABLE 2 -- SUMMARY OF MODELING RESULTS
FOR PANTHER BRANCH

STORM DATE	STATION	PEAK FLOW OBS. cfs	COMP. cfs	RUNOFF VOLUME OBS. 10^6cu.ft.	COMP. 10^6cu.ft.
10/28/74	P-10	342	360	24.40	29.03
	P-30	376	410	39.34	36.16
11/10/74	P-10	979	600	64.48	53.44
	P-30	897	705	72.87	73.61
11/24/74	P-10	680	645	52.24	57.72
	P-30	774	735	73.70	78.97
12/05/74	P-10	273	315	36.06	32.66
	P-30	329	370	45.52	48.55
12/10/74	P-10	464	380	44.42	33.61
	P-30	517	425	51.73	43.02

The 3.42 sq mi of drainage area upstream of Station H-20 was divided into 24 subcatchments with an average size of 91 acres. Physical parameters were determined in a manner similar to that for Stations P-10 and P-30. The infiltration parameters and the observed and computed peak flows and volumes at Stations H-10 and H-20 are listed in Tables 3 and 4, respectively. The observed and computed hydrograph and suspended solids pollutograph for the storm of 5/08/74 at Station H-20 are shown in Figure 6. During the initial phases of the modeling program it was determined that due to testing difficulties, BOD_5 modeling could not be verified.

As seen in Figures 4, 5, and 6, the computed hydrographs are reasonably acceptable, but the suspended solids pollutographs for urban areas are severely deficient. Other investigators have arrived at a similar conclusion[6].

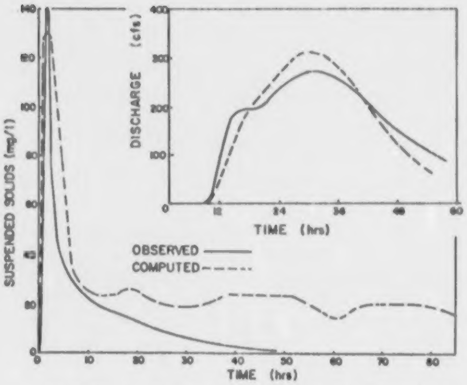

FIGURE 4--GAGE P-10, STORM OF 12/05/74

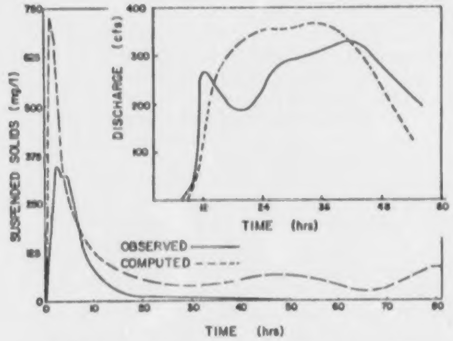

FIGURE 5--GAGE P-30, STORM OF 12/05/74

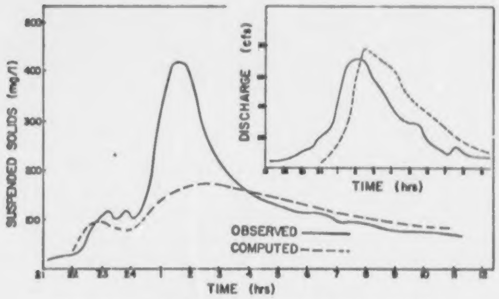

FIGURE 6--GAGE H-20, STORM OF 5/08/74

Future Directions

The modifications and additions to the SWMM which are discussed in this paper indicate that the modeling of storm water runoff quantity by the SWMM has been considerably improved. The new infiltration and baseflow models allow a closer parallel to the observed hydrograph.

The modeling of smaller subcatchment areas with more definitive hydrologic regimes will provide a method of evaluation of the capabilities of the new subroutines and computational methods in the SWMM. This type of data are presently being accumulated in The Woodlands.

Storm water quality modeling in the SWMM is constantly being improved but the results are still less than satisfactory as shown in the preceding section. The present size and structure of the SWMM limits the application of the new methodology described in this paper. Therefore, it is expected that any significant improvement in water quality modeling by the SWMM will necessitate a complete revision of the present methodology.

TABLE 3 -- INFILTRATION PARAMETERS FOR HUNTING BAYOU WATERSHED

STORM DATE	STATION	INFILTRATION RATES Initial in/hr	Final in/hr	Decay /sec
9/08/68	H-10	1.00	0.10	.0005
	H-20	1.00	0.10	.0005
9/17/68	H-10	0.75	0.10	.0005
	H-20	0.75	0.10	.0005
11/09/70	H-10	2.50	0.10	.0005
	H-20	2.50	0.10	.0005
3/26/74	H-20	0.10	0.02	.0005
5/08/75	H-20	0.30	0.10	.0005

TABLE 4 -- SUMMARY OF MODELING RESULTS FOR HUNTING BAYOU

STORM DATE	STATION	PEAK FLOW		RUNOFF VOLUME	
		OBS. cfs	COMP. cfs	OBS. 10^6cu ft	COMP. 10^6cu ft
9/08/68	H-10	121	160	1.43	1.85
	H-20	325	355	4.48	4.69
9/17/68	H-10	144	155	2.82	2.24
	H-20	333	365	8.37	6.02
11/09/70	H-10	85	125	1.50	0.97
	H-20	161	220	3.50	2.65
3/26/74	H-20	40	38	1.46	1.93
5/08/75	H-20	73	80	1.38	1.32

In conclusion, the SWMM has been a valuable tool in determining the storm water runoff characteristics of The Woodlands. The quantity of flow has been predicted satisfactorily and the quality of flow from undisturbed areas is also satisfactory. The modeling of quality of flow from disturbed areas is very complex and further detailed data and study are necessary.

Acknowledgements

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MODELING IN SOLID WASTE MANAGEMENT: A STATE-OF-THE-ART REVIEW

David H. Marks
Professor of Civil Engineering
Room 1-163
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Summary

The application of modeling for the prediction of cause and effect relationships for policy change and for the analysis of decisions in choosing policy levels in solid waste management is discussed in five major subsystems: 1) the organization of individual collection systems (routing, scheduling, distributing, crew assignment; 2) the choice of collection technology; 3) the organization of city-wide or regional systems (facility location); 4) the choice of process and disposal technology; 5) estimation of waste generation for short-term and long-term policy changes. Selected listings of models in each area and an appraisal of the transfer of modeling to practice are presented as well.

Introduction

The large scale system by which residential solid waste is generated, stored, collected, transported, processed, recovered and disposed of is a complicated and expensive system to successfully manage. There are many points within the system where policy decisions about the types of technology used, level of service offered and organization of services provided can be made which can strongly effect the cost of the system as well as impacts on other important objectives such as environmental quality. However, there has been only moderate success in gaining an overall perspective of decision possibilities. For a detailed discussion of structure of the solid waste management system and our level of knowledge about cause and effect relationships in each component, the recently completed National Science Foundation study on Solid Waste Management (Hudson, et al, 1974) is suggested. The purpose of this paper is to provide some order and summary of analytic methods available for gaining insights about policy decisions to be made in the system. The word model is used to imply the representation of a complex real phenomena by a conceptual analog which is easier to manipulate to gain understanding about the real system. Generally in application, such models take two forms: predictive models and decision models. Predictive models are used to gain insight about the magnitude and direction of changes in system performance measures brought about by changes in policy variables. While it is possible in theory to derive such models for Solid Waste Management inductively from assumptions of the basic underlying mechanisms of the system, most predictive models are deductive. That is, based on observed data taken on system variables and outputs, relationships are built usually using statistical techniques or for more complex systems simulation. Decision models on the other hand assume a knowledge of the underlying cause and effect relationships between policy variables and system output and attempt to address the choice of level of policy variables based on their impacts on stated objectives. Such models are optimization techniques such as linear programming, dynamic programming, or search. Throughout the discussion of models in this paper, the tradeoffs between the detailed nature of the model and the cost of data and solution, as well as the acceptability of the assumptions of the theoretical model in real practice must always be kept in mind.

Modeling activity in the field of environmental activities over the last few years has been extensive, and solid waste management has been no exception. While the development of the computer and its introduction as a routine tool of practice in engineering has been an important motivating factor in the design and adoption of models to aid management, not all modeling efforts need to be computer based as will be shown later. Further, a complex model may be more difficult to transfer than a simple one. To present in these few briefly allowed pages some overview and assessment of the types of problems in solid waste management where models have been developed, the paper will be structured by presenting major subsystems and the modeling work appropriate to each. An apology is made in advance that due to space and time limitation, the author has selected only five major topics, where considerable work has been done, although there is evidence of work in others. Also, with each major topic, either because of lack of space or lack of knowledge of all possible contributions, not all modeling work done in that area has been presented. The five major areas discussed are: The organization of individual collection systems (routing, scheduling, crew assignment), The choice of collection technology, The organization of city-wide or regional systems (facility location problems), The choice and design of process technology, and Estimates of waste generation for short-term and long-range planning. This is followed by an appraisal of how well these models have transferred from development to application. In general, the success of transfer has not been great because of the general difficulty encountered in several areas. One is that a strong enough effort to transfer these models from academic and governmental research groups to actual practioners has not been make nor is such a transfer easily designed. Even more important, many of the models are not general enough to transfer easily or require huge amounts of data that are expensive to collect. Finally, many of the decision models are based on regional cost and do not realistically address other important issues such as subarea cost and impact distribution.

Models for Organizing Local Collection Systems

Models for dividing up communities into tasks for individual crews, and for efficiently routing the crews over the street network have been developed by a number of researchers. The work is applicable to almost any collection system, and seems to be both complete and thorough.

The routing problem for solid waste collection is actually a combination of a large number of problems, each of which can be solved with reasonable effort. At one level, "routing" involves taking the area to be collected by a crew on a day, and finding an efficient path which will enable them to do the collection with the least travelling. Another side of "routing" involves deciding which crew should collect from what set of demands, and dividing up the work to be done into task assignments. Shuster and Schur (1974) call the former problem microrouting and the latter districting or route-balancing;

this seems to be a reasonable terminology. Microrouting generally takes two forms. A *node-routing problem* involves an attempt to pick up waste from a set of fixed points, while travelling the least. In the literature, this is often referred to as the "travelling-salesman problem" or the "trick-dispatching problem" when many trucks are used. An *arc-routing problem* involves travelling down all the streets, collecting whatever is there, and again attempting to minimize the amount of travel. This problem is known as the "Chinese Postman's Problem," or the "m-postmen's problem" for the case with more than one route at a time.

In any routing study, the decision of what makes a reasonable route is the important first stage. Routes should require an equal amount of work, where possible, and some method must be available for choosing a fair assignment. The choice of such a fair day's work is closely related to waste generation (see later section in this paper), topography and demography, productivity, level of service, and the trade-off between overtime and incentive time. If the estimation of the work required to collect individual blocks is poor, than it will be impossible to form balanced task assignments, and the routing study will be useless. The best compendium of methods for estimating work involved in collection is that by Shuster (1973). Shell and Shupe (1973) also discuss this issue. Hudson (1975) describes the use of census data, which are readily available, for estimating waste generation and collection time. Lofy (1971) has developed a simple model for the task-balancing problem which attempts to minimize lost time at the end of the day.

Districting or Route Balancing

Several methods have been proposed for taking the data on the work required in any specific area and converting these work requirements into routes. These methods may be computerized (see Hudson, 1973), but they may also be manual. Shuster (1973) discusses manual procedures for this method in detail.

Microrouting

The problem of microrouting is how to take a set of districts, and generate detailed collection routes from them, minimizing mileage and left-hand turns, going the correct way on one-way streets and grades, and meeting other similar objectives.

Shuster and Schur (1974) develop a manual method for reducing the number of left-hand turns in a route, by making clockwise (right-hand) loops whenever possible.

More advanced methods of minimizing mileage in collection have been developed by Stricker, (1971), Hudson, et al (1973) and by Liebman and Male (1973). The M.I.T. approach involves manual routing techniques, preceded by districting; the basic output is the choice of which streets should be traveled twice and which only once, to minimize travel. The approach developed by Liebman is somewhat different. Analysis is done first on how mileage in collection can be minimized for the whole collection area. Then the whole collection area is subdivided into balanced districts and rerouted.

For all practical applications, the node-routing problem reduces to an application of the Clark and Wright algorithm developed about 12 years ago (1964). There are other techniques available, but the Clarke and Wright approach is both easy to understand, and available in packaged form from most computer companies (e.g., IBM's VSP — Vehicle Scheduling Program (1968). It can also be applied by hand fairly easily. Beltrami and Bodin (1974) have extended the basic algorithm to problems involving containers with different frequencies of collection, such as schools and restaurants on the same route, with some success. The Clark and Wright algorithm does not work well if the starting and ending points of the route are widely separated, but route modification after the analysis is fairly easy.

Several companies have developed and marketed routing packages and have made claims of tremendous savings. In a well managed moderate sized system, some savings can probably be realized by the implementation of these methods. However, claims of large savings from computerized routing usually include all savings from the major redesign of an inefficient system. The actual amount saved by the modeling procedures are probably smaller.

For crew scheduling, Bodin (1972), Heller, et al (1973), and Ignall, et al (1972) have proposed models for making shift and day assignments. Lofty (1971) proposes a model for assigning crews to routes based on their productivity.

Models for Choice of Collection Technology

Research on the choice of vehicles for collection has concentrated on the issues of truck capacity and age of replacement. Techniques have been developed for choosing vehicle capacity to minimize cost, and for estimating the age at which a truck should be replaced. Degner (1971) presents a detailed breakdown of vehicle costs by a variety of measures such as capacity, turning radius, type of loading, etc. After listing and analyzing all these attributes, his work provides about the only available detailed discussion of a method for choosing a particular type of vehicle out of the available set of packer bodies and chassis manufactured. The technique used is DARE, (Decision Alternative Ration Evaluation) which is a performance scoring tool: a number of objectives are stated, along with their relative importance to the decision-maker. Then the available choices are evaluated according to the objectives, and a generalized score is created, giving information about which is best. See Klee (1970) for a good description of the DARE technique. Clark and Helms (1972) develop a model for choice of vehicle size using data from Buffalo. They relate capacity to cost and residences served per truck per day and use an optimization technique to solve for truck size. A similar model is proposed by Cardile and Verhoff (1974). Clark and Gillean (1974) developed a simulation model to test system configurations in terms of truck capacity and crew size for Cleveland. Quon, et al (1970) presents a model to show the effect of truck age on collection efficiency. Douglas (1973), and Degner (1971) also consider models for estimating the economic life of a collection vehicle.

The Organization of City-Wide or Regional Systems

At issue here is an evaluation of where facilities for transfer and processing should be located and what form they should take, as well as the assignment of subareas to facilities. Most of the techniques provided for this task are optimization models based on minimization of regional cost of facilities and transportation. There are numerous examples such as Hekimian (1973), Berman (1974), Weston (1973), Fuertes, et al (1974), Helms and Clark (1970), Morse and Roth (1970), Marks and Liebman (1971), Skelly (1968), Schultz (1968), Wersan, et al (1971), and Vasan (1974). The two papers on the EPA SWAMP program for regional solid waste management presented at this conference are based on the Skelly model. Table 1 gives a comparison of the models according to what factors are included in costs and the type of optimization techniques used for solution.

Minimization of total cost is not, however, the only objective in planning solid waste management systems. Local costs allocation and impacts are also important but not considered.

Currently, a major effort is underway in systems analysis research on models to include social and political objectives with a least cost economic analysis. Examples are Fuertes, et al (1974), Kuhner, et al (1974) and Hekimian (1973). Klee (1971) developed DISCUS, a solid waste management game which is capable of calculating total transfer, transportation, processing and disposal costs for a given system design. This is used in an interactive process to help decision makers aware of the tradeoffs involved in different decisions about the system.

Numerous other simulation models of city-wide organization are available including Truitt, et al (1969), and Wersan (1965).

Models for the Choice and Design of Processes

Methods exist whereby the alternative processing options may be evaluated so that the least-cost alternative can be selected. Unfortunately, the cost data available, especially on the relatively new processes, are often tentative, limited, or unreliable.

One method for ranking alternatives is DARE (Decision Alternative Ration Evaluation) developed by Klee (1970). The process requires the user to make a number of comparisons between pairs of different evaluating criteria in order to develop a weighting system for those criteria. This provides the ability to establish a uniform scoring procedure for all alternatives. It has also been applied for collection technology as previously noted.

Another approach is to use mathematical programming techniques in order to minimize the net present cost of establishing a processing facility. Such a model has been developed by Clark (1972). Clark's model can provide an estimate of what a facility will cost over time including borrowing costs for facility construction, assuming the model given is fair representation of the taxing, borrowing, and spending policies currently in municipal practice.

Wenger and Rhyner (1972) and Popovich, et al (1973) use a cost-effectiveness analysis approach to evaluate solid waste disposal systems. Essentially, this involved first stating a set of objectives for the system and then ranking the various candidate alternatives according to this set of objectives.

Models for Estimating Waste Generation

The prediction of the quantity and composition of solid waste is important both for short-term planning such as route design and for long-term facility planning and technology choice. The first type of model is concerned with the detailed local prediction of quantities expected per collection. Alpern (1972) developed a model using Los Angeles data relating waste production to housing type, income and topography. Hudson (1975) uses aggregate cross-section data to investigate waste load changes with changes in system policies such as frequency of collection and place of collection, as does Quon (1968). McFarland (1972) did simular work for income level, Clark and Toftner (1972) worked from land use (zoning) data and DeGeare and Ongerth (1971) describe commercial establishments. Long range modeling is more difficult. Stern (1973) uses an input output methodology for industrial waste generation as does Steiker (1973).

Having described these models for different management subcategories, it is important to consider how well they have been transferred to real use in local and regional planning. There are considerable barriers to model transfer in environmental planning which must be carefully accounted for and eased before tools such as these will be widely used. One important barrier is that most of these models have been developed without much input from the users. Thus, while they may be of academic interest, they address the wrong problem or do not give enough information about the most important aspects to the local users. A good example are the regional least cost facility location models which promise to choose the optimal system configuration for solid waste facilities from among feasible sites on the basis of facility and transportation costs. To most local planners, the high external costs (real or imagined) of such facilities make no site feasible because of local opposition. Thus, they do not seek optimal location but any location where they can build the facility. Mention has been made of improving optimality criteria for such models to include social factors which may be one way out of this dilemma. But a better way might be through considerable interaction with the local planner to see what information he can use to help design plans that have a broad base of public support and, therefore, can be implemented. At a minimum, this would include an estimate of disaggregated local impacts. Such interaction is not easy nor inexpensive. Considerable time must be spent in establishing a good dialogue between theoreticians who think in terms of models and computers and local planners who are possibly distrustful of them. We have been guilty in the past of over selling the computer as a panacea that could automate planning procedures and solve all our problems. However, the tools developed just can't and probably won't ever capture all the nuances of a specific application. For truck routing algorithms, it is hard to input to models that some crews are better performers than others or that some streets are hard to access from particular directions. Thus, we must be more careful to emphasize the use of models to aid our intuition about the problem and to educate planners about system tradeoffs. With local users as partners in the development and fine tuning of models to real use, transfer can take place. It might well be necessary to work through a rather lengthy local case study with each local area to which the model is to be transferred before such tools will be widely used.

In summary, I feel at this point in time that theoretical development must be focused on the task of producing with interaction from local planners on simple to use models which can use readily available data and produce information focused on specific local situations. More elegant algorithms developed without local input are not needed at this point and doomed to gather dust on the shelf and in the journals without much chance of implementation. Rather focusing on issues such as impact prediction, assessment of objectives of local interest groups and means for showing graphically what the inherent conflict is between differing objectives for the solid waste system will make a more positive step toward better model application.

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Requirements	Simulation Model Many Authors	Hekimian	Berman	Weston	Fuertes, et al	Helms & Clark	Moorse & Roth	Marks & Liebman	Skelly, M.J.	Baker, J.S.	SERL	Schultz	Wersan, S. et al	Vasan	Authorship
Aggregate Generation			X	X	X		X	X	X		X		X	X	
Household Generation		X				X				X		X			
Haul Distances		X	X	X	X	X	X	X	X	X			X	X	
Coordinates											X	X			
Linear Haul Costs		X	X	X		X	X	X	X	X	X			X	
Haul Cost Functions					X							X			
Facility Capacities		X				X	X		X			X		X	
Limits on Capacity			X	X	X			X						X	
Linear Operating Costs		X					X				X				
Operating Cost Functions			X	X	X	X		X				X		X	
Given Haul Routes						X			X	X					
Reduction Factors			X	X	X		X							X	
Fixed Costs		X	X	X	X	X		X	X					X	
Growth Rates		X	X		X							X			
Limitations															
Local Optimum	X	X	X	X	X	X			X	X		X			
Limited Alternatives	X	X	X		X	X	X	X	X		X	X		X	
Linear Costs	?	X					X						X		
Short-Term	X			X		X	X	X	X	X	X		X	X	
No Capacity Limit	?									X	X		X		
Well Defined System	X					X		X				X			
Capital Costs	?						X			X	X	X	X		
Extensive Data Input	X		X		X							X		X	
Development			X	X								X			
Weak	X					X	X			X		X			
Probable Application	X	X		X									X		

TABLE 1: COMPARISON OF LEAST-COST FACILITY LOCATION TECHNIQUES

WRAP: A MODEL FOR REGIONAL SOLID WASTE MANAGEMENT PLANNING

Edward B. Berman
The MITRE Corporation
Bedford, Massachusetts 01730

Summary

An optimizing model called WRAP (Waste Resources Allocation Program) has been developed for the generation of minimum cost regional solid waste management plans.

This model is addressed to the state, regional, and local planner who is responsible for sorting out the confusing array of alternatives available to him, and for finding a solution which is both economically viable and politically acceptable.

The model was originally designed in eighteen alternative modes of operation (nine static modes and nine dynamic modes) under a MITRE sponsored research project.[1] WRAP is a fixed-charge linear programming model, using an algorithm developed by Dr. Warren Walker.[2]

In 1974, a basic static mode of the model was used for a program of operational runs in support of regional design analysis for the Commonwealth of Massachusetts. This program used manually-generated inputs to the algorithm, and a manual interpretation of outputs.[3]

The Office of Solid Waste Management Programs, U.S. Environmental Protection Agency, has supported the further development of the model. The EPA program includes:

- the development of a computerized front end and back end for one static mode and one dynamic mode of the model;
- an operational test program on the Greater St. Louis Region (the City of St. Louis and seven surrounding counties);
- a parametric exercise program on a region of 53 communities of Massachusetts and New Hampshire; and
- documentation and dissemination.

This paper describes the model in brief and the philosophy of its application programs. The focus of the discussion is on the use of the model to illuminate political and technical issues, using the original Massachusetts application as an example. The paper concludes with a description of a model improvement program now underway at MITRE.

The following paper by Ms. Donna M. Krabbe of EPA describes an analytical evaluation of the St. Louis operational test program.

Background

Economies of scale available from two processes from the point of view of a potential processing site in Haverhill, Massachusetts are illustrated in figures 1 and 2. The costs are based on MITRE preliminary haul and processing costs for the two processes. Note that the decline in processing costs in Figure 1 compensates for rising haul costs as the region is enlarged, and the minimum cost available is attained at the maximum region size considered, including all 14 zones (representing 53 communities and 3600 TPD).

In figure 2, there are less economies of scale available, so that the minimum cost is obtained with the inclusion of only 4 zones (representing 20 communities and 1700 TPD).

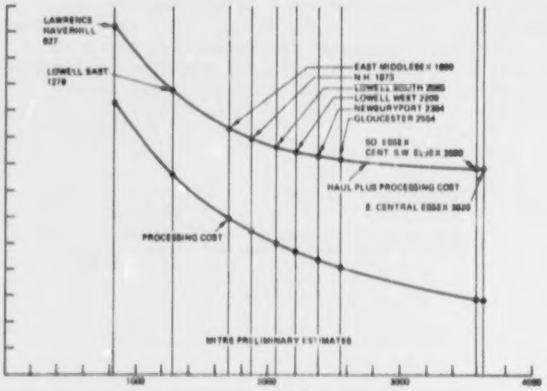


Figure 1. Economies of Scale in Dried Shredded Fuel/Residue Recovery

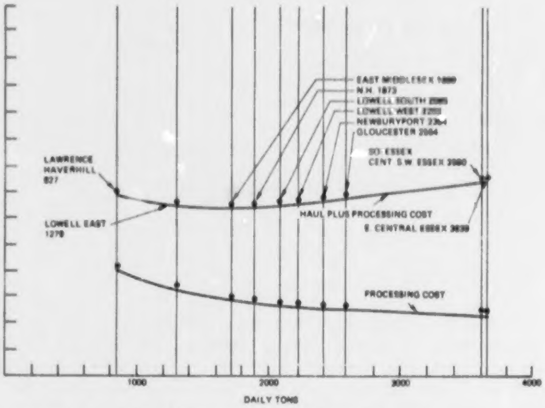


Figure 2. Economies of Scale in Gas Pyrolysis (MITRE Preliminary Estimates)

Economies of scale in processing are a driving force towards regionalization, but from regionalization two problems are generated:

- a complexity of system design, and
- a problem of political consensus.

WRAP is addressed to both of these problems. It is intended to:

- sort out the many alternatives on siting, sizing, linking, and process selection for transfer stations, primary processing, secondary processing, and disposal; and to generate the minimum cost plan which will meet all requirements; and

- illuminate political issues and hence help their resolution.

Brief Description of the Model

Figure 3 presents an overview of the model, its inputs and its outputs. Note that both fixed and variable costs are input. The output is a comprehensive regional solid waste management plan, including the selection of sites for transfer, processing, and disposal, the selection of a process at each site, the sizing of each site, and the selection of links and flows connecting sources, transfer sites, processing sites, and disposal sites. The plan is preferred in the sense that it is the minimum cost plan that meets all requirements, given the sites, processes, and links that were made available.

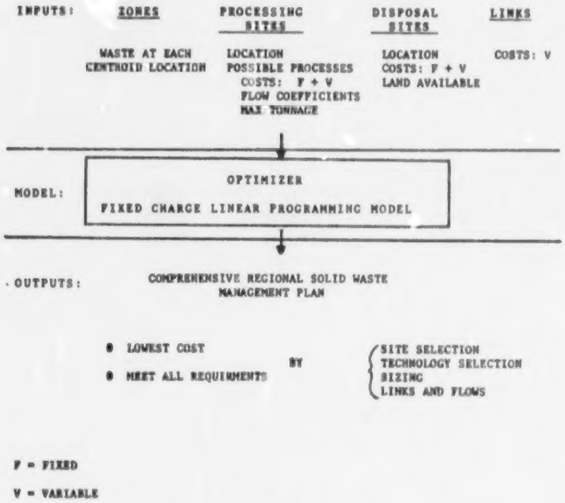

INPUTS:
ZONES
PROCESSING SITES
DISPOSAL SITES
LINKS
WASTE AT EACH CENTROID LOCATION
LOCATION
POSSIBLE PROCESSES
COSTS: F + V
FLOW COEFFICIENTS
MAX TONNAGE
LOCATION
COSTS: F + V
LAND AVAILABLE
COSTS: V
MODEL:
OPTIMIZER
FIXED CHARGE LINEAR PROGRAMMING MODEL
OUTPUTS:
COMPREHENSIVE REGIONAL SOLID WASTE MANAGEMENT PLAN
● LOWEST COST
● MEET ALL REQUIREMENTS
BY
SITE SELECTION
TECHNOLOGY SELECTION
SIZING
LINKS AND FLOWS
F = FIXED
V = VARIABLE

Figure 3. Model Overview

Figure 4 describes the five levels in the model and allowable linkages among levels. Note that linkage from one A-level process to another A-level process is permitted. In the St. Louis application, this capability was used to allow a packer-to-van transfer process to link to a truck-to-rail transfer process. Similarly the dual C-level capability permits the model to carry two differential residue commodities (incinerator residue and air classification heavy-end) into secondary processing through dummy secondary recovery processes in which differentiated revenues are generated. This capability was used in the Massachusetts/New Hampshire exercise program.

LEVEL	LINKAGE TO
SOURCE	A, B, D
A. TRANSFER STATION	A, B, D
B. PRIMARY PROCESSING	C D
C. SECONDARY PROCESSING	C D
D. SANITARY LANDFILL	—

Figure 4. Model: Levels of Processing

A key capability of the model is its ability to trade off the economies of scale in processing, obtainable through centralized processing, as against the haul costs implied by such centralization. Essential to this trade-off capability is the ability to represent economies of scale in process costs. Figure 5 illustrates a concave total cost function, typical of solid waste processing, as represented by several linear segments. Since the model is cost-minimizing, it will seek out the lowest cost segment at any level of tonnage. Thus the capability of treating cost in two parameters (fixed and variable, or intercept and slope) permits the model to represent economies of scale at any level of accuracy desired. In the actual WRAP applications, three-segment representations have been used for nearly all processes.

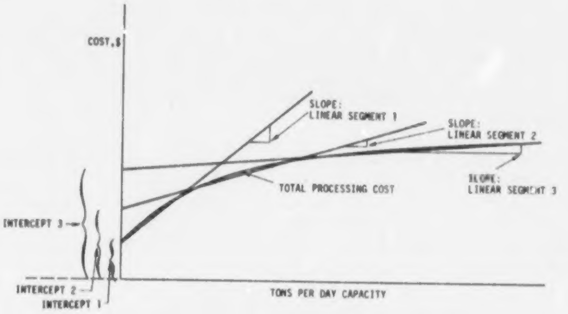


Figure 5. Piecewise Linear Approximation of a Concave Function (Representing Economies of Scale)

The model has three essential components:

Structure - which assures that each alternative considered is feasible, handles all wastes, processes all residues, and so forth;

Cost - which assures that each alternative is properly costed, including economies of scale where appropriate; and

Procedure - which is an organized search for the best solution.

Figure 6 illustrates the operation of the model. The basic structure is rectangular, which means that there are more variables than equations, and hence that the problem is underdetermined. Thus there are many solutions. Among the many solutions to the system of equations, only that subset of solutions which have no negative solution values is considered to be feasible (for a negative solution value implies grinding up the outputs of the process and generating its inputs). The optimal solution is that particular feasible solution which is lowest in cost.

The structure is a system of equations that assures that each of the solutions examined is feasible in the sense that (1) all wastes generated are entered into transportation; (2) all wastes arriving at a site are processed; (3) all residues generated are processed at the site or entered into transportation; and (4) no process exceeds indicated tonnage maximums.

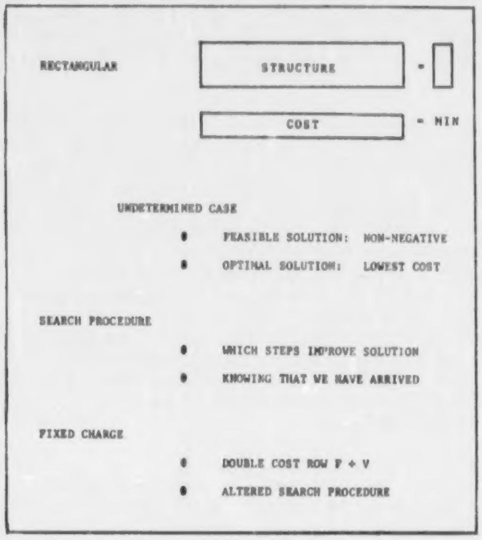

RECTANGULAR
STRUCTURE
=
COST
= MIN
UNDETERMINED CASE
• FEASIBLE SOLUTION: NON-NEGATIVE
• OPTIMAL SOLUTION: LOWEST COST
SEARCH PROCEDURE
• WHICH STEPS IMPROVE SOLUTION
• KNOWING THAT WE HAVE ARRIVED
FIXED CHARGE
• DOUBLE COST ROW F + V
• ALTERED SEARCH PROCEDURE

Figure 6. Operation of the Model

The search procedure requires:

- that those steps which improve the solution can be separated from those that make it worse; and

- that the procedure knows when it can go no further (i.e., when it has arrived at the optimum).

The "steps" are transitions from one feasible solution to another.

In the fixed-charge linear programming procedure, the algorithm adds the fixed cost (to the system cost) whenever the corresponding solution value goes from zero to positive, and subtracts the fixed cost whenever the corresponding solution value goes from positive to zero. The fixed-charge algorithm considers both fixed and variable costs in determining whether a transition is an improvement.

The fixed-charge algorithm also requires one or another kind of forcing to make sure that the solution domain is searched out thoroughly, thus avoiding a "local optimum" solution. This step is unnecessary in standard linear programming, in which there are no local optima. The operational runs of WRAP have used "single forcing," in which each column outside of the solution is forced in, and the new solution is evaluated for improvement over the best previous solution. The Walker algorithm also includes a double forcing procedure in which all possible pairs of columns outside of the solution are forced in, and the new solution evaluated for improvement; but this procedure is practical only for very small problems. A new "group" forcing procedure has been designed, and is described in the final section of this paper.

Applications: Illuminating Political and Technical Issues

An application, which is a set of runs, is designed to illuminate political and technical issues.

Each run in the set will:

- handle all wastes,
- meet all environmental standards (since only processes which do meet relevant standards are offered),
- provide the lowest cost solution for its "case."

The "case" is a defined state of political/technical feasibility. WRAP will generate a plan and a system cost for each case. The incremental costs of moving from case to case are calculated, and in particular the costs of moving from less political acceptability to greater political acceptability. Figure 7 illustrates a hypothetical plan set.

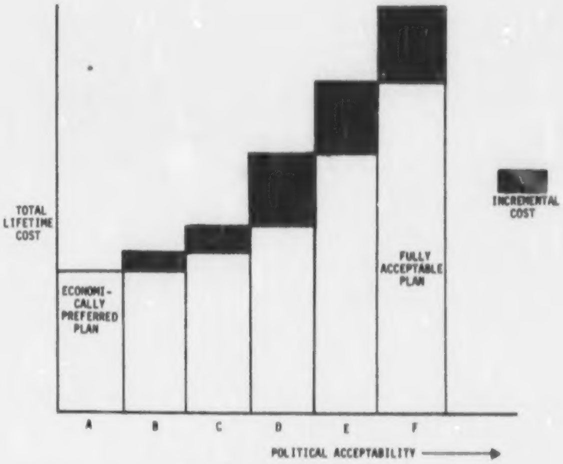


Figure 7. The Plan Set

Figure 8 summarizes issues which have been illuminated in the three applications which have been completed at this writing.

- REGION SIZE
  - MASS: LARGE REGION: HOW DOES IT BREAK DOWN
  - ST. LOUIS: REGION VS STATE - BY - STATE
- PROCESS AVAILABILITY
  - POLITICAL
    LANDFILL IN MASS. & ST. LOUIS
  - TECHNICAL
    GAS PYROLYSIS IN MASS.
- SITE AVAILABILITY
  - ST. LOUIS - PROCESSING AT PLANT
  - MASS. - SOUTH ESSEX SITE
- MARKET AVAILABILITY
  - ST. LOUIS - ILLINOIS POWER CO.
- SENSITIVITY
  - TONNAGE, MARKET PRICES, PROCESS COSTS

Figure 8. Illumination of Issues

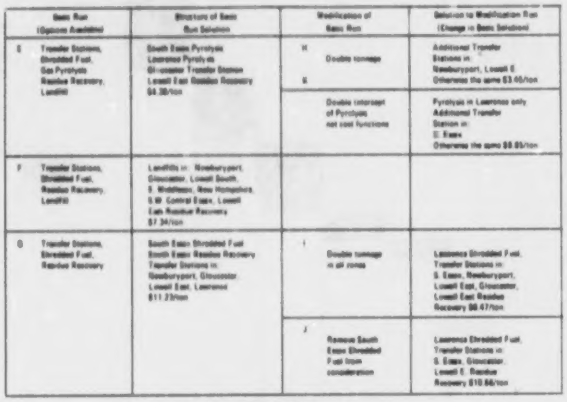
The Massachusetts Application

A region of 47 communities in Northeastern Massachusetts and 6 in New Hampshire was evaluated primarily to determine how the region would break down under varying circumstances. The region was divided into 13 zones for tonnage generation.

Process options were transfer station, dried shredded fuel, gas pyrolysis, sanitary landfill, and residue recovery.

The residue recovery process in Lowell East was given a reduction in all intercept costs of $634.1 per day to represent the amortized value of an EPA grant which was obtainable only if that process was selected at that location.

The seven basic runs in the Masschusetts application, runs E through K, are described in Figure 9. (Runs A through D were experimental.)



Basic Run (Options Available)	Structure of Basic Run Solution	Modification of Basic Run	Solution to Modification Run (Change in Basic Solution)
E Transfer Stations, Shredded Fuel, Gas Pyrolysis Residue Recovery, Landfill	South Essex Pyrolysis Lawrence Pyrolysis Gloucester Transfer Station Lowell East Residue Recovery [illegible]/ton	H Double tonnage	Additional Transfer Stations in Newburyport, Lowell E Otherwise the same [illegible]/ton
		K Double intercept of Pyrolysis net cost functions	Pyrolysis in Lawrence only Additional Transfer Station in E. Essex Otherwise the same [illegible]/ton
F Transfer Stations, Shredded Fuel, Residue Recovery, Landfill	Landfills in: Newburyport, Gloucester, Lowell South, S. Middlesex, New Hampshire, S.W. Central Essex, Lowell East Residue Recovery $7.34/ton		
G Transfer Stations, Shredded Fuel, Residue Recovery	South Essex Shredded Fuel South Essex Residue Recovery Transfer Stations in Newburyport, Gloucester Lowell East, Lawrence $11.23/ton	I Double tonnage in all zones	Lawrence Shredded Fuel, Transfer Stations in S. Essex, Newburyport, Lowell East, Gloucester, Lowell East Residue Recovery $8.47/ton
		J Remove South Essex Shredded Fuel from consideration	Lawrence Shredded Fuel, Transfer Stations in S. Essex, Gloucester, Lowell E. Residue Recovery [illegible]/ton

Figure 9. Summary of Massachusetts Runs

Note that:

- with all options (run E) gas pyrolysis was selected in two locations;
- with gas pyrolysis removed (run F) landfill was selected in six locations for an incremental $3 per ton (gas pyrolysis was not quite in the state-of-the-art as of the time of the analysis);
- with landfill removed (run G) (it is of questionable political acceptability in Northeastern Massachusetts) shredded fuel was selected in one location for an incremental $4 per ton (or an incremental $3.50 per ton with a Lawrence location as in run J); and
- doubling the pyrolysis intercept (run K) reduced the number of processing locations from two to one, and added a transfer station.

Ms. Krabbe will present an analytical evaluation of the St. Louis operational test in the following paper.

The Massachusetts exercise program has been described in an earlier paper.[4]

Model Improvement Program

As the EPA-supported model development program neared completion, opportunities for improvement of WRAP were identifed. MITRE internal funds have been made available for the initiation of two of these, as follows:

- A marketing version of WRAP, called RAMP (Recovery and Market Planning Model) has been designed and carried through initial development, a stage in which it can be used by MITRE in its operational solid waste planning work. The model has been run several times in support of a an ongoing planning study for the Commonwealth of Massachusetts. RAMP provides a marketing capability, with multiple commodities, multiple market locations, and multiple marketing segments, with upper bounds. The model traces the effects of market saturation, and determines the impact on the preferred solution that results therefrom. RAMP generates specific transportation activities linking the various processing centers with the various markets.
- An improved forcing procedure called "group forcing" has been designed, and program specifications for it have been developed. Group forcing will take advantage of the structural features of WRAP and RAMP to generate a better solution (i.e., a reduced probability of a local optimum) in less running time. An essential aspect of group forcing is the necessity to define forcing groups of columns which are adjacent extreme points relative to one another; and it is this aspect of the technique that is model-specific (i.e., relates to WRAP and RAMP only). Forcing groups will be forced both in and out, whereas the Walker Algorithm forces in only, and only one or two columns at a time.

Through use of group forcing, it will be possible to explore the solution domain with both greater effectiveness and less running time.

The two improvements together should provide a substantial improvement in the capability to define preferred solutions to real problems.

Notes

1. This design was reported in MITRE Report M73-111, Edward B. Berman, A Model for Selecting, Sizing, and Locating Regional Solid Waste Processing and Disposal Facilities, October 1973.

2. Warren Walker, Adjacent Extreme Point Algorithms for the Fixed Charge Problems, Dept. of Operations Research, College of Engineering, Cornell University, January 30, 1968.

3. The runs were reported in , Edward B. Berman and Harold J. Yaffe, MITRE Report MTR-2945, Regional Design Analysis for Regional Resource Recovery System for Northeastern Massachusetts, November 1974.

4. Edward B. Berman and William M. Stein, The MITRE Solid Waste Management Planning Model: A Status Report, Presented at the Sixth Annual Northeastern Regional Antipollution Conference, College of Engineering, University of Rhode Island, July 8-9, 1975. A MITRE report by the author, WRAP - A Model for Regional Solid Waste Management Planning: Documentation of Operational and Exercise Runs, is in final stages of preparation.

ST. LOUIS: AN APPLICATION OF WRAP

Donna M. Krabbe
Operations Research Analyst
Office of Solid Waste Management Programs
U.S. Environmental Protection Agency
Washington, D.C. 20460

ABSTRACT

A mathematical model called WRAP, Waste Resources Allocation Program, was developed to aid regional solid waste planners in sorting through the myriad of problems and possible solutions that they find confronting them. The true purpose of the model is not to find the optimum solution, but to use it to find a structured series of solutions which will clearly show the impact of decisions made concerning major issues.

This paper discusses the series of model runs done for the East-West Gateway Coordinating Committee to illuminate some of the major issues confronting the decision makers in the St. Louis area.

BACKGROUND

States, regions, counties, cities and towns across the country are facing critical questions about what to do with solid waste. How can we plan systems that dispose of these wastes? Which of the many disposal options is the best? Which will meet environmental objectives as well as provide the least expensive solution? These questions are particularly difficult to answer when a plan must be developed for a region consisting of a number of municipalities, a large area, and a complex transportation network.

Many options are available today, or are rapidly emerging for consideration. In addition to new techniques in landfilling and incineration, there are numerous resource recovery technologies, which can, for example, process mixed waste to produce energy products like steam or dry fuel as well as recover additional materials for marketing. Within the next several years, more technologies will become available.

Each of these technologies has distinct economic advantages and disadvantages, and the suitability to a particular area is dependent upon a number of factors. Among these are the existence and proximity of markets for the various reclaimed products, the existence of sufficient amounts of waste to warrant a particular processing technology and to utilize the economies of scale inherent in that process, and the availability of land.

The array of options is confusing yet decision makers must be informed about the full system cost of the major options available to them. Most importantly, decision makers must be able to determine the economic effects of varying and changing elements of the system, according to specific desires and needs.

A computer model called WRAP, Waste Resources Allocation Program, has been developed in order to assist decision makers with these and other complicated considerations. The model enables its users to sort out all the various options and generate and cost a number of solid waste management plans. Plans are expressed in terms of location and capacity of sites and processes, and the total flow of waste in the transportation network. Total annual cost of the system and cost per ton are computed. One of the most important features of the model is that it can be used to guide the decision making process in the selection of alternative systems and translate the impact of this selection into cost figures.

APPLICATION OF WRAP

Although WRAP is an economic, optimizing model, its power lies not in selecting the solution for a regional area, but in allowing a decision maker to analyze the impact of his decisions. This is accomplished by structuring and executing a series of runs which will induce the model to react to changes of basic assumptions or decisions by generating and costing an alternate set of plans. The incremental cost of one plan over another is the cost of that decision or change of conditions.

What this approach to WRAP offers is an effective combination of optimization and gaming. One uses the model iteratively to examine issues and decisions (gaming) but at each step many options can be made available, with the best combination being selected (optimization).

ST. LOUIS

Under the sponsorship of the Office of Solid Waste Management Programs, the model was applied to identify and illuminate issues in Greater St. Louis, where the Union Electric Co. is proposing to install an 8,000 ton per day resource recovery system using the shredded fuel process developed by them. The proposed system included the marketing of the recovered fuel to Union Electric's power generating stations within Greater St. Louis. A local regional planning agency, the East-West Gateway Coordinating Council, requested EPA to fund an application of the model to provide further insights into the advantages to the communities of participating in such a plan.

WRAP IN ST. LOUIS

Preparation of the WRAP application was a joint effort among the East-West Gateway Coordinating Council, the Union Electric Co., the Mitre Corporation and EPA.

The WRAP model was used to analyze the 450 square mile area of Greater St. Louis, encompassing 185 municipalities, and roughly two and one-half million people, producing an estimated 8,000 tons per day of residential, commercial and industrial waste. 185 landfills and dumps, and two incinerators currently provide inadequate disposal services to the area, often in violation of environmental regulations. The Union Electric Company is proposing a large resource recovery system using the shredded fuel process (shredding, air classification, magnetic separation of ferrous metals) developed by them, including the marketing of the fuel to Union Electric's steam generating stations within the region.

THE ISSUES

The solid waste planners at the East-West Gateway Coordinating Council identified the following primary issues which needed to be investigated:

1) Will the Union Electric shredded fuel process be competitive with landfill?

2) Should processing for shredded fuel be at the utility sites or at other locations?

3) What would be the impact of restrictions upon interstate flow of refuse and and shredded fuel?

4) What would be the effect of the loss of the Illinois Power company as a potential market?

5) How would a refusal by some large commercial haulers to participate affect the system?

SETTING UP THE APPLICATION

Data for the application was drawn largely from an earlier report prepared for the East-West Gateway Coordinating Council. The data comprised costs of the proposed Union Electric process, the Bureau of Mines residue recovery process, transfer stations, landfills, and truck and rail haul, as well as revenues from the sale of recovered material and energy, and waste generation rates. The region was divided into 29 districts for waste generation and possible transfer and processing sites were located.

Structuring of the model runs was, of course, the critical step in obtaining insight about the issues to be examined. The number and purpose of the runs needs to be defined in order to give structure to the analysis process, but the modeler must remain flexible about eliminating and adding runs dynamically as the runs progress.

Originally six runs were anticipated for the St. Louis problem. During the course of the analysis, one run was dropped as irrelevant, but three more were added to examine collateral issues. These runs are listed in Table 1.

Table 1. Summary of St. Louis Runs

A	Base Case (Off-Site)	$1.253 per ton
A-1	B. C. with rail haul	1.440 per ton
B	Landfill available	1.249 per ton
B-1	L. A. with rail haul	1.610 per ton
C	No Interstate Flow	1.840 per ton
D	Loss of Illinois Power	Not Run
E	Reduced Tonnage	1.750 per ton
F	On-Site Processing	1.950 per ton
F-1	On-Site Expanded	1.590 per ton

For each of the above runs, WRAP generated a solution consisting of system costs, process and site selections, and transportation activities.

ANSWERS TO ISSUES

Is Shredded Fuel Competitive with Landfill?

This first question is answered by a comparison of the A and B runs. The cost of a total resource recovery system (Run A) is $1.253 per ton. When landfill was offered (Run B), it was selected to handle only .5% of the waste of the entire region and cost was reduced by only $.004 per ton.

The systems selected in A and B were almost identical and were off-site processing for shredded fuel. Included in these runs was the assumption that fuel produced at off-utility sites would be trucked to the closest utility location from each site that was chosen for processing. The solutions in A and B resulted in all of the fuel being trucked to the same utility site (there are two in the region), exceeding the capacity of that site. This then raised a collateral issue of the method of haul for fuel produced off-site.

Should Fuel Be Hauled by Truck or Rail?

Runs A-1 and B-1 were added to the planned series of runs to correct the capacitation problem of A and B by changing the truck haul of fuel to rail haul. This change did indeed have the desired effect. Rail haul caused the waste to be sent to both utility sites. Comparison of the A-1 and B-1 runs show that the availability of landfill does not benefit the region. We can safely conclude that resource recovery is competitive with landfill for the region.

Should Processing Be At The Utility Sites?

This question is really answered by the fact that the base case (A-1) which offers both on-site and off-site processing selected off-site processing. What, then, would be the incremental cost of on-site processing? To answer this question Run F was used to force a selection of on-site processing. Cost increased by $.51 per ton. The solution in F, however, showed a curious selection of only one utility site for shredded fuel processing. Thus, another issue was raised.

Should Only One Utility Site Be Used for Shredded Fuel Processing?

The utility site which was not selected in Run F was actually closer to many of the waste centers, but it was constrained to a maximum input of 2,000 tons per day of raw refuse. Was this capacitation constraint the cause of its rejection? What would happen if it was expanded? Run F-1 raised the constraint to slightly more than 4,000 tons per day. The result was the selection of processing at that site at full capacity with the remainder of waste going to the second utility site, and a cost reduction of $.36 per ton.

The comparison of F and F-1 tells us that enough transport cost can be saved to justify the capital expenditure at the first utility site if the capacity is at least 4,000 tons per day, but not if the size of the facility is too greatly restricted (i.e., 2,000 tons per day). The fact that the model selected full utilization of the facility also indicates that greater savings might be achieved if it were expanded further.

Because F-1 has a more desirable solution than F, it should be used in answering the question of on-site vs. off-site processing. Comparison of A-1 and F-1 show, of course, that off-site processing is still more desirable, and that the cost of on-site processing is $.15 greater than off-site processing. Figures 1 and 2 show the geographical ramification of the on-site/off-site controversy. Both flows from generation point to initial offload point, and the transfer network of flow from initial offload point are shown.

Figures 3 and 4 depict the comparison of on-site processing at one site only and the better system of processing at both sites.

What Impact Would Interstate Restriction Have?

The impact of interstate restictions on the flow of refuse was assessed by comparing Run C with the base case (A-1). There was no interstate transport of raw refuse in the base case solution, so the changes in the system and the incremental cost, $.40 per ton, are the result of the restriction on transport of primary processing residue which had to be shipped to a central secondary processing site in Missouri. The secondary process is beneficial enough that the model decided to construct a facility for this process in both Missouri and Illinois when residue flow was restricted.

What Would Be The Effect of Only One Market for Shredded Fuel?

In the base case run, the model had available to it markets both in Missouri (Union Electric) and Illinois (Illinois Power). The model selected only use of the Missouri market and, therefore, this question is irrelevant.

What Effect Would A Drastic Change in Volume of Raw Refuse have on the System?

To examine the impact of a reduction of raw refuse entering into the system, Run E was designed. Such a question is relevant because much of the waste in the region is controlled by large private collection companies. It is essential to know what impact their nonparticipation, for whatever reason, would have upon the system. Comparison of the Run E solution to the base case indicates that the location of primary processing should be shifted further out from the city center if less waste is anticipated. This is due to the fact that much of the waste to be lost would be the commercial waste concentrated in the downtown business centers. Loss of of this waste would increase the system cost $.31 per ton.

CONCLUSION

Perhaps one of the greatest insights obtained by using WRAP in the St. Louis region is that the incremental cost of most decisions is going to be small compared to experiences of other areas in the country. The model shows the decision makers that they can have a great deal of flexibility in reordering the design of their system when confronted with unchangeable real-world situations. For intance if off-site processing is unacceptable to the community, on-site processing is a viable alternative for only a $.15 per ton higher cost. While all of the unfavorable alternatives and constraints examined for the region increase the cost of operation, none has so drastic an effect that it mandates radical changes or abandonment of the resource recovery system planned. This provides decision makers with the required framework in which to confidently proceed in the final design of a workable solid waste management system.

The work in the St. Louis area illustrates how WRAP can be used effectively to sort out the best solutions from a staggering array of possibilities. Decisions that would oftentimes be made on political considerations can be based on solid analytical techniques when using such a sophisticated tool. A model such as WRAP can help decision makers discover the best, minimum cost system, as well as the cost of deviating from that system. Realization of the true impact of their decisions will lead decision makers to wiser choices.

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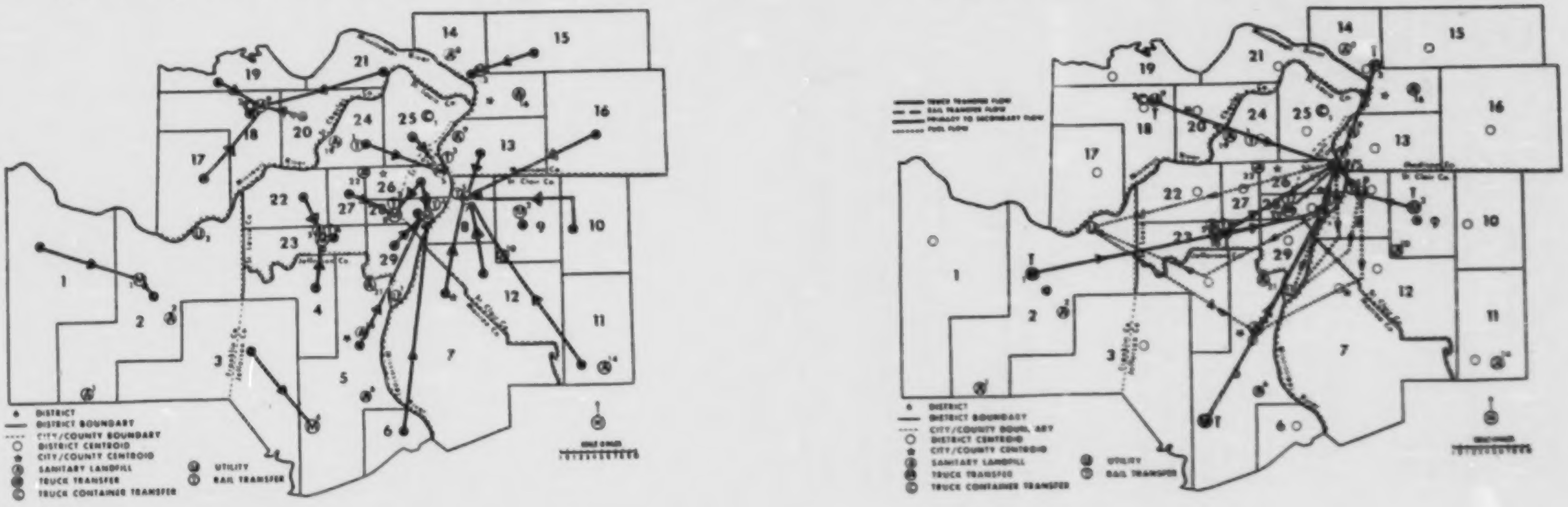


FIGURE 1: SHREDDED FUEL PROCESS: OFF UTILITY SITE

$1.44 PER TON

FLOWS TO INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN A-1

FLOWS FROM INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN A-1

DISTRICT
DISTRICT BOUNDARY
CITY/COUNTY BOUNDARY
DISTRICT CENTROID
CITY/COUNTY CENTROID
SANITARY LANDFILL
TRUCK TRANSFER
TRUCK CONTAINER TRANSFER
UTILITY
RAIL TRANSFER
TRUCK TRANSFER FLOW
RAIL TRANSFER FLOW
PRIMARY TO SECONDARY FLOW
FUEL FLOW
St. Clair Co.

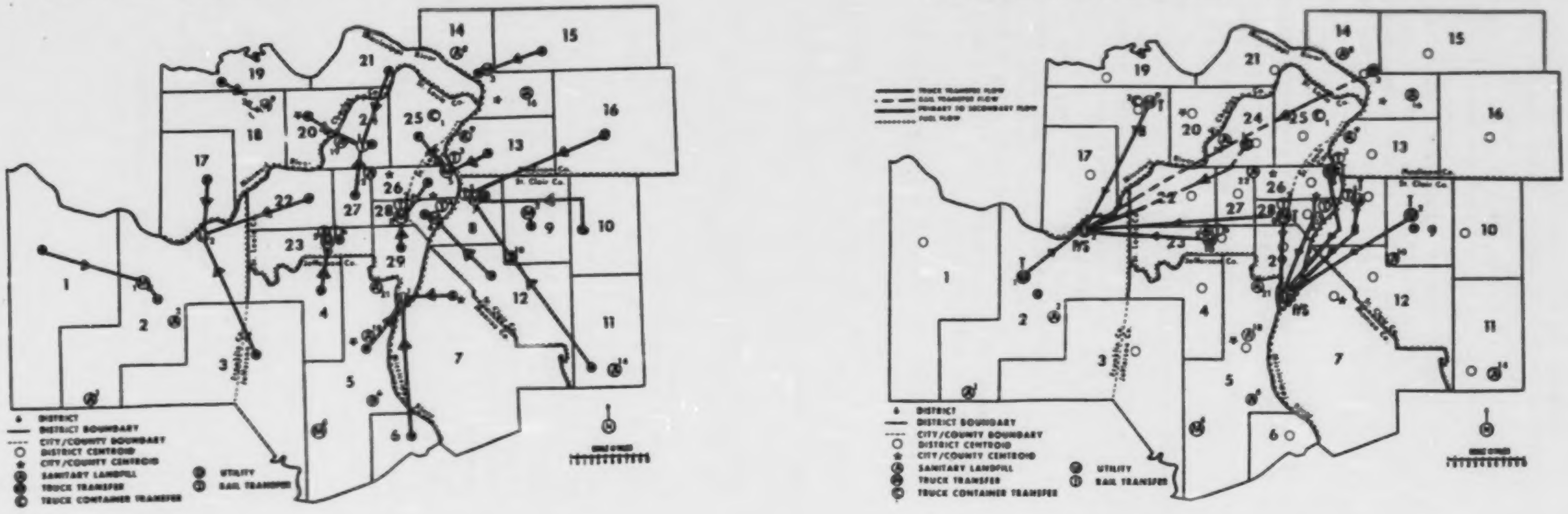


FIGURE 2: SHREDDED FUEL PROCESS: ON UTILITY SITE

$1.59 PER TON

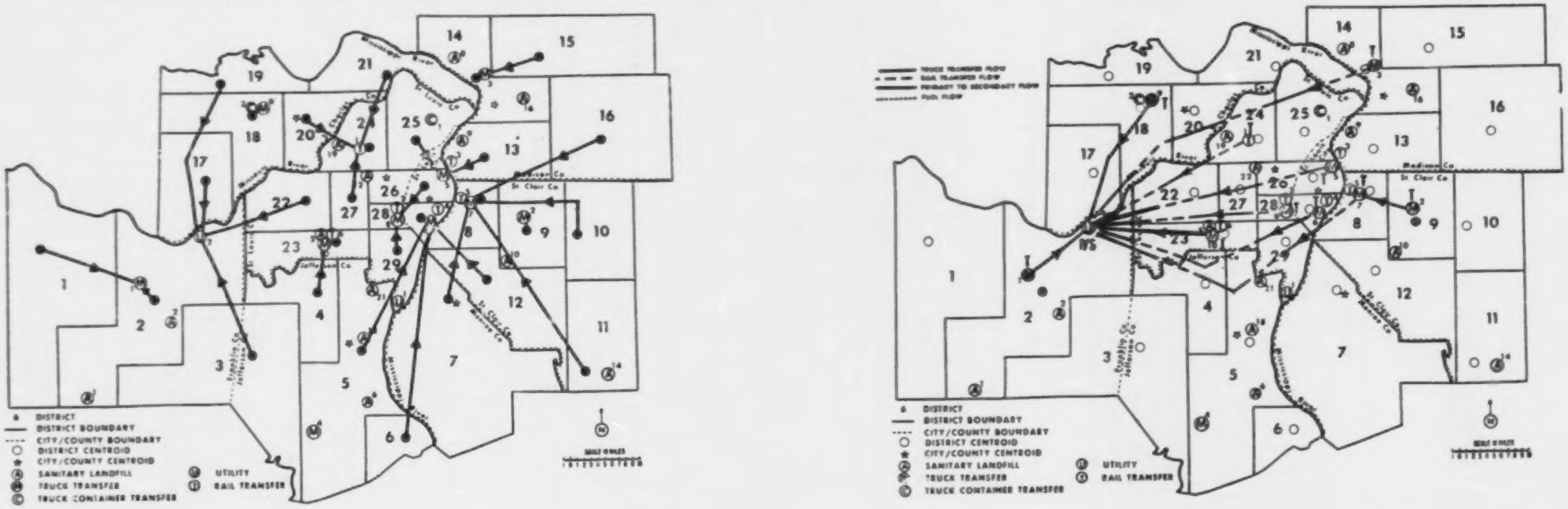
FLOWS TO INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN F-1

FLOWS FROM INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN F-1

DISTRICT
DISTRICT BOUNDARY
CITY/COUNTY BOUNDARY
DISTRICT CENTROID
CITY/COUNTY CENTROID
SANITARY LANDFILL
TRUCK TRANSFER
TRUCK CONTAINER TRANSFER
UTILITY
RAIL TRANSFER
TRUCK TRANSFER FLOW
RAIL TRANSFER FLOW
PRIMARY TO SECONDARY FLOW
FUEL FLOW
St. Clair Co.

FIGURE 3: CAPACITY CONSTRAINED AT MERAMEC (U.)

$1.95 PER TON



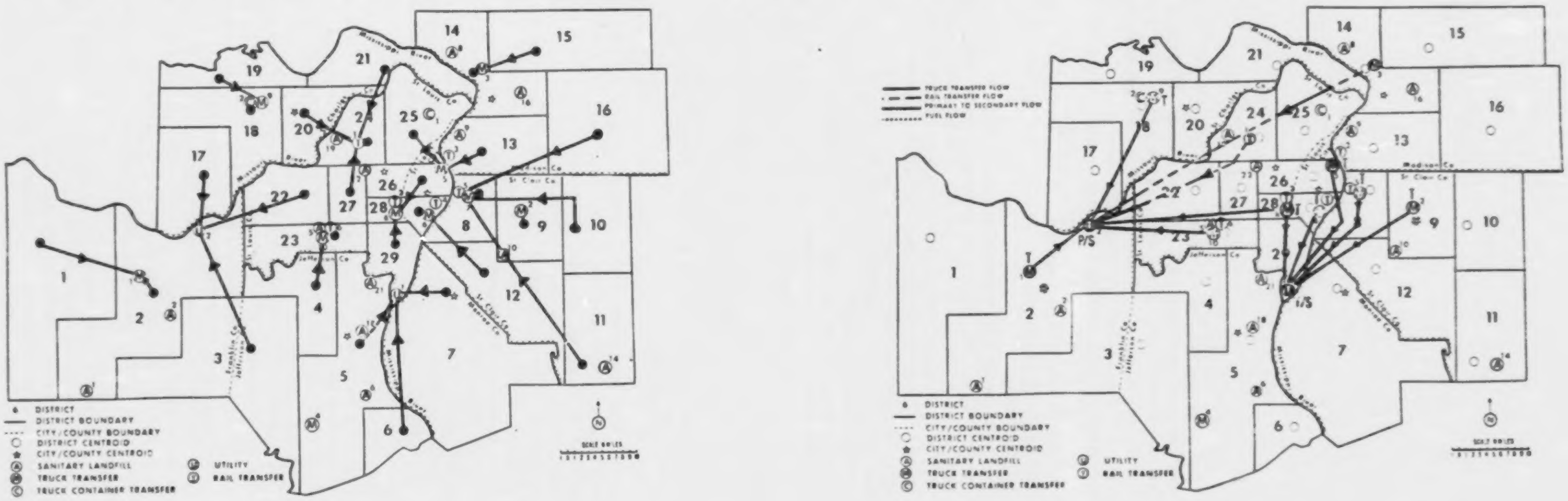
FLOWS TO INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN F

FLOWS FROM INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN F

TRUCK TRANSFER FLOW
RAIL TRANSFER FLOW
PRIMARY TO SECONDARY FLOW
FUEL FLOW
DISTRICT
DISTRICT BOUNDARY
CITY/COUNTY BOUNDARY
DISTRICT CENTROID
CITY/COUNTY CENTROID
SANITARY LANDFILL
TRUCK TRANSFER
TRUCK CONTAINER TRANSFER
UTILITY
RAIL TRANSFER
SCALE-MILES
St. Louis Co.
Madison Co.
St. Clair Co.
Monroe Co.
Jefferson Co.
Franklin Co.
Mississippi River
P/S

FIGURE 4: CAPACITY EXPANDED AT MERAMEC (U.)

$1.59 PER TON



FLOWS TO INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN F-1

FLOWS FROM INITIAL OFFLOAD POINT : THE ST. LOUIS REGION, RUN F-1

TRUCK TRANSFER FLOW
RAIL TRANSFER FLOW
PRIMARY TO SECONDARY FLOW
FUEL FLOW
DISTRICT
DISTRICT BOUNDARY
CITY/COUNTY BOUNDARY
DISTRICT CENTROID
CITY/COUNTY CENTROID
SANITARY LANDFILL
TRUCK TRANSFER
TRUCK CONTAINER TRANSFER
UTILITY
RAIL TRANSFER
SCALE-MILES
St. Louis Co.
Madison Co.
St. Clair Co.
Monroe Co.
Jefferson Co.
Franklin Co.
P/S
I/S

DEVELOPMENT OF A MODEL FOR AN ORGANIC SOLID WASTE STABILIZATION PROCESS ON A PILOT PLANT

D.S. Whang
Division of Water Resources
New Jersey Department of Environmental Protection
Trenton, New Jersey

G.F. Meenaghan
Office of Research Services
Texas Tech University
Lubbock, Texas

Abstract

The expansion of commercial production of fed cattle has resulted in a severe source of pollution and hazard to health. The bio-stabilization of organic solid waste is one of the few disposal processes which recover the organic fraction of the wastes. In spite of the potential value of this process, lack of engineering information has hindered its utilization and application. For this reason, an investigation was instituted to ascertain the kinetic and generalized model of the system.

A small pilot plant was used for the purpose of this study. The data obtained from this unit was analyzed with a computer model called COMPOST. The result of this analysis and modeling indicated that the behavior of bio-stabilization model was consistent with the reaction model of forming an intermediate organism-substrate complex under a quasi-equilibrium condition. A mathematical model of the overall process was developed, which could be used for optimizing the design of the process. The culmination of this research resulted in the development of a system model which predicts the behavior of the bio-stabilization process. The kinetic model obtained may be used as a model to study the bio-stabilization process on an industrial scale. Particular attention should be devoted to scale-up factors for industrial application.

Introduction

The treatment and disposal of waste from the operation of livestock industry has come to the fore as a matter of considerable importance in pollution control. The problem is attributable to the increasing concentration and quantity resulting from the mass production of fed cattle. There are two major factors that must be considered in attempting to solve a pollution problem: a treatment process must be economically feasible for operation and it must satisfy the conservational criteria for the receiving environment. As emphasized by the Federal legislation concerning solid waste management, the ideal scheme of a pollution control process would be ultimate recycling of all wastes generated.[1] The bio-stabilization of the organic wastes, commonly called composting, is an excellent example of a pollution control process which recycles wastes.

Even though the composting has a long history in its application, there is no published work in the area of the kinetics and modeling of the process which, from a chemical engineering point of view, may be a controlling factor in the design and optimization of the process. Once the kinetic behavior of the process has been defined, a mathematical model for the overall system could be used for the optimization of the entire process.

A small composting pilot plant was used to obtain the kinetic data for this study. The enzymatic kinetic theory has been applied for the analysis of the kinetic data obtained. A mathematical model for the system has been developed and verified using the results of the kinetic analysis to simulate the bio-stabilization process of the organic waste treatment. The purpose of this investigation was to ascertain a kinetic model of an organic solid waste stabilization process and to develop a generalized system model in an attempt to provide rational information for the optimization of the process.

Theoretical Considerations

The Optimum Reaction Conditions

Approximately half of all urban wastes and some industrial wastes can be bio-stabilized to a sanitary, humus-like material.[2] As the reaction proceeds, the causative organisms use nutrients in the organic wastes and develop all of the protoplasm and energy necessary for the metabolism. Approximately one-third of the carbon in the organic wastes serves as a source of energy. The conversion of the substrates into energy causes a rise in temperature. The magnitude of the temperature rise is an indication of the intensity of the microbial activity, accelerating the reaction rate.

The activity of the micro-organisms is highly dependent upon the environmental conditions to which they are subjected. Among these are temperature, moisture, pH, aeration and nutrients.[3] The optimum temperature range for most cases has been found to be 50 to 70° C. It has been known that aerobic assimilation can occur at any moisture content between 30 and 100 percent. Aeration can be used to reduce excess moisture in the decomposing material and at the same time provide the required oxygen for the microbial activity. Particle size also effects the efficiency of the aeration. Among the elemental requirements of nutrients, carbon and nitrogen are of major concern, especially the carbon to nitrogen ratio.[4]

The end product of the bio-stabilization is a humus material by which the organic wastes are returned to the ecological cycle in a productive form. The organic wastes usually consist of carbon, hydrogen, nitrogen and oxygen. Despite the differences in reaction mechanisms, the overall reaction is similar to that of a catalyzed oxidation reaction of organic elements.

Development of the System Equations

The enzymatic kinetic theory, developed by Michaelis and Menten,[5] has been applied for the development of a system equation, i.e.

$$r = \frac{k_2 c}{k_1 + c} \tag{1}$$

where,

k_1 = kinetic constant
r = reaction rate
c = concentration of substrate.

On the other hand, based on an inert material, namely ash, and for a batch operation of the system under consideration (see Figure 1), a material balance of the substrate for the system results in the following equation:

$$wr = \frac{d(wc)}{dt} \qquad (2)$$

where,

w = weight of ash in the system
t = time.

Combining Equations (1) and (2), since w is a time-independent constant in the system, one obtains

$$\frac{dc}{dt} = \frac{k_2 c}{k_1 + c} \qquad (3)$$

The initial condition of the Equation (3) is $c(0) = c_o$. Solving Equation (3) using the initial condition,

$$t = \frac{k_1}{k_2} \ln\left(\frac{c}{c_o}\right) + \frac{1}{k_2}\,(c - c_o) \qquad (4)$$

Equation (4) completely defines the behavior of the system under consideration if the kinetic constants, k_1 and k_2, are known.

Transformation of the System Equation

If one defines the dimensionless time and concentration as follows:[6]

$$Z = \frac{k_2}{k_1}\,t \qquad (5)$$

and

$$Y(Z) = \frac{c}{c_o} \qquad (6)$$

Then, the initial condition, $c(0) = c_o$, becomes

$$Y(0) = 1 \qquad (7)$$

and Equation (4) becomes

$$Z = \ln Y + \frac{c_o}{k_1}\,(Y - 1) \qquad (8)$$

Equation (8) is a dimensionless system equation with a dimensionless initial condition, Equation (7). This equation competely describes the behavior of the compost system under investigation.

Experimentation

Description of the Pilot Plant

A small pilot plant as shown in Figure 1 was used for the purpose of this investigation. The pilot plant consisted of an oxygen supply system, a humidifier, and a reactor. Humidified air was supplied to the reactor by a perforated pipe which was attached to the bottom of the reactor. The reactor was insulated with a coating of Eagle Pitcher cement to prevent biological energy loss. The reactor was rotated by a gear-reduction-motor to provide mixing and aeration of the reactants.

An opening was made on the top of the reactor to facilitate manual filling and emptying of the reactant material. An exhaust port welded onto this opening provided access to the inside of the reactor for the sampling for the elemental analysis of carbon. The maximum capacity of the pilot plant was 60 kilograms per batch.

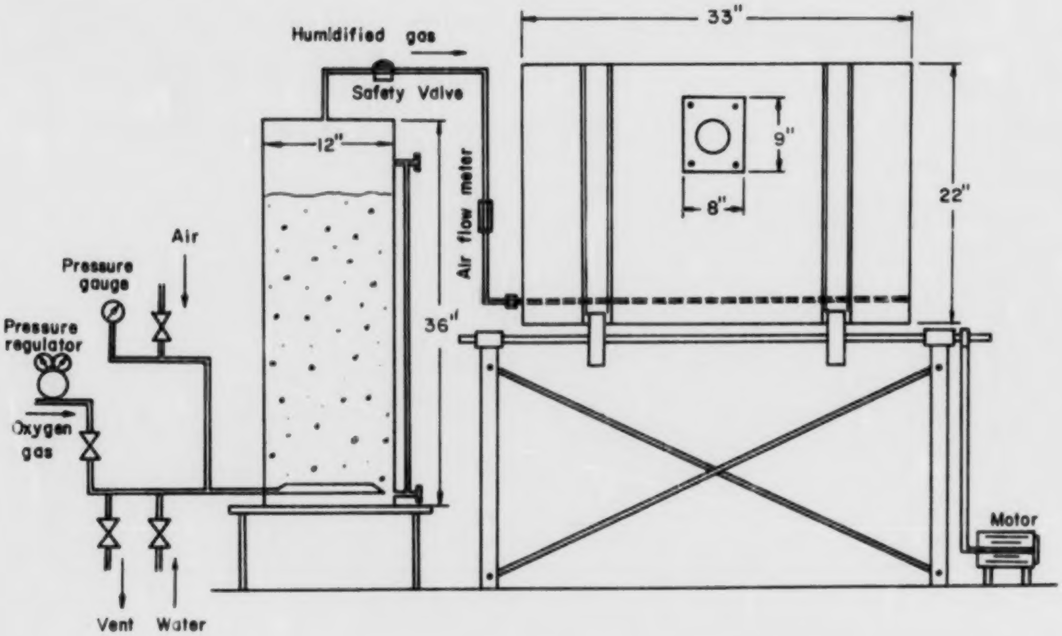


Figure 1. The Pilot Plant

Raw Material

Cattle manure from the Texas Tech University Experimental feedlot was used as the raw material for this investigation. In general, the fresh manure contained 85 percent moisture and 15 percent volatile and fixed solids. Grab samples from the surface of the feedlot were directly loaded to the reactor. The age of the manure ranged from three to ten days.

Chemical Analysis

Grab samples were taken from the reactor to analyze the change of elemental carbon concentration with respect to time. A CHN analyzer, Model 185, manufactured by Hewlett Packard, Avondale, Pennsylvania, was used to analyze carbon content of the samples. The content of carbon, measured as grams of carbon per gram of ash, was used as a system parameter for the development of the system model.

The samples for chemical analysis were dried in a Bleeder-Vacuum chamber under a vacuum of 20" mercury at a room temperature for 72 hours. The dried samples crushed to 48 mesh for the analysis. Cyclohexane 2, 4-dinitrophenylhydrazone (C_6H_{10}:N.NH.$C_6H_3(NO_2)_2$) was used as a standard reference sample to provide calibration data.

Operating Conditions

Samples were loaded manually to the reactor through the opening. The sample weight ranged from 34.5 kg to 49.5 kg. The supply gas for oxygen was saturated with water. The pilot plant reactor was turned one to three times every day to provide proper mixing and aeration of the reactants. All experiments were conducted on a batch basis. A summary of the operating conditions of the experimental scheme is shown in Table 1.

Table 1. The Operating Conditions of Reactor for the Stabilization Reaction

Experiment No.	4	5	6
Sample weight, kg	49.5	34.5	34.5
Source of oxygen	Air	Oxy.	Oxy.
Frequency of mixing, per day	1	3	1
Gas flow rate, l/min	3	6	6
Moisture, percent	63	52	52

Results and Discussion

The results of the chemical analysis and the change of carbon concentration with respect to time are shown in Figure 2. The reaction rates were determined by measuring the tangent of the curve for each experiment. The "symmetric mirror technique" has been applied to measure this tangent. The kinetic constants, k_1 of Equation (1), may be determined by the application of the Lineweaver-Burke method.[5] The Lineweaver-Burke plot involves transforming Equation (1) into the following form and the kinetic constants are determined graphically using the paired values of 1/r *vs.* 1/c:

$$\frac{1}{r} = \left(\frac{k_1}{k_2}\right)\frac{1}{c} + \frac{1}{k_2} \qquad (9)$$

In this analysis, a regression technique has been

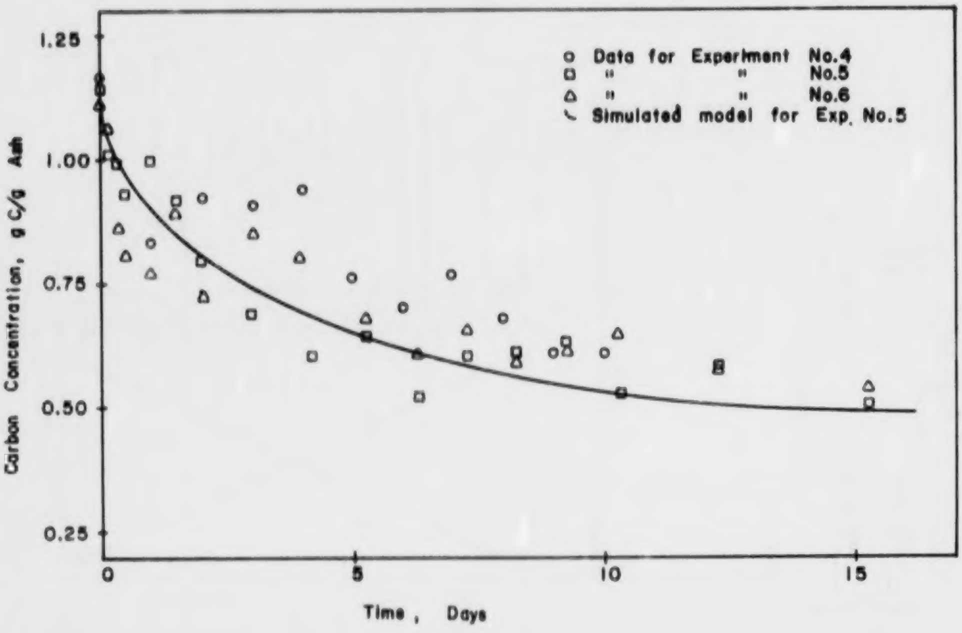


Figure 2. Experimental Data and Simulated Model

used to preclude human prejudice in the determination of the values of k_1. The results of this analysis, which was obtained from a subroutine of a main computer program, are summarized in Table 2.

Table 2. Kinetic Constants of the Proposed Kinetic Model

Experiment No.	4	5	6
k_1, g C/g Ash	1.062	1.136	1.224
k_2, g C/g Ash-day	0.011	0.033	0.029

A computer simulation model of the system, called COMPOST, has been developed and used for the processing of all experimental data obtained for this investigation.[7] The COMPOST enables to predict the behavior of the bio-stabilization system during the decomposition of the material. One advantage of the model is its capability to describe the system behavior in a dimensionless form. This generalization of the model in system analysis may be directly applicable to scale-up of the process.

In Equation (3), k_1 is a dissociation constant of an enzyme-substrate complex and is a measure of the affinity of the enzyme for the substrate. As shown in Table 2, all values of k_1 found in this investigation have the same order of magnitude within experimental error range while those obtained for k_2 vary considerably depending on the experimental conditions. The consistency of k_1 in magnitude indirectly verifies that k_1 is a characteristic constant of the system. An increase in the magnitude of k_2 would result in a higher reaction rate. Its contribution to the reaction rate is directly proportional to its magnitude.

It should be noted that approximately 300 percent increase was found in the magnitude of k_2 when pure oxygen was used as the oxygen source. This increase compares favorably with the data reported for the activated sludge process in which the process was found to be more effective.[8] It should be noted, however, that the magnitude of k_1 in this study was independent of the oxygen source.

The system equation, Equation (4), was developed based on the mass balance and Michaelis-Menten kinetic theory. The curve in Figure 2, which simulates the behavior of the system during the decomposition reaction, is a plot of Equation (4) using kinetic constants given in Table 2 for Experiment No. 5. As can be seen from the figure, the mathematical model is consistent within the experimental error range.

Equations (5) and (6) define dimensionless time and concentration, respectively. The use of dimensionless variables allowed for the system to be interpreted more easily. Figure 3 shows the results of these transformations. It should be noted that the slope of the curve depends upon the initial concentration only as can be seen from the Equation (8). It was expected that the type of the curve is similar to that of the curve in Figure 2.

The system model may provide basic analytical information for control and optimization of the process for commercial application. However, the control of the bio-stabilization process is still based on experience due to lack of analytical information in the design procedure. Further investigation may be necessary for optimizing the entire process in industrial application. The kinetic data and model herein reported should be used as a model to study the bio-stabilization process on an industrial scale. Particular attention should be devoted to scale-up factors from pilot scale to industrial operation. In conclusion, the proposed model does predict the behavior of the system.

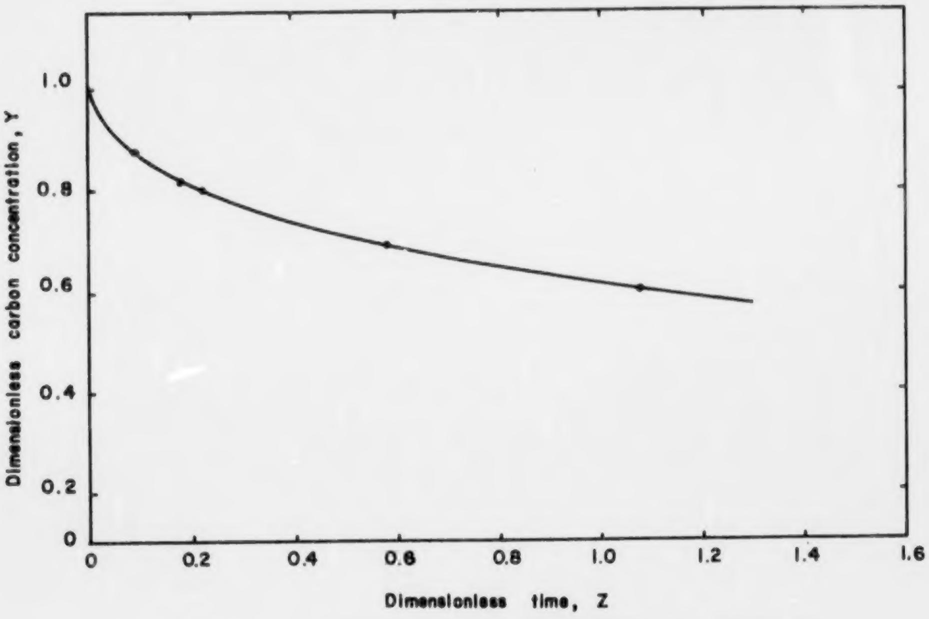


Figure 3. Change of Carbon Concentration with Respect to Time in Dimensionless Form for Experiment No. 5

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EVALUATION AND SELECTION OF WATER QUALITY MODELS: A PLANNER'S GUIDE

E. John Finnemore and G. Paul Grimsrud
Systems Control, Inc.
Palo Alto, California

Summary

As part of a management guide for planners,[1] Systems Control, Inc., recently developed for the Environmental Protection Agency systematic procedures for evaluating and selecting receiving water quality models. Using these procedures, each model is evaluated on the basis of many considerations, which include both the technical principles and capabilities of the models and such resource needs and constraints as additional labor, specialized technical expertise, time and funds, and computer limitations. All these considerations are combined into a single performance index. A procedure is also prescribed for combining the various component costs of applying the model into a single overall cost. A comparison of this overall application cost with the model's performance index may then be used as a guide to model selection. The selection procedure is organized into phases of increasing level of detail, each of which may or may not be required depending upon the nature of the planning problem being confronted.

Background

The priority given to the accomplishment of the nation's commitment to the goal of clean water is evidenced by the size of the investment being made for abatement and prevention of water pollution. This commitment makes management decisions affective receiving water quality of the utmost importance. With such major decisions being made daily as part of numerous planning programs, it is incumbent on planners to assure that the expenditures they recommend are justified and that the courses adopted will fully achieve the expected results.

But the selection of water quality planning methodologies, one of the first major decisions facing planners and managers, requires a good understanding of the difficult technical problems which may be involved, besides the limitations of time and funds.

Since the number of wastewater management alternatives which exist and require evaluation may be large, the complexity of water quality analysis has stimulated the development of a variety of tools to assist planning, ranging from simple graphical techniques to sophisticated computerized models. While these tools frequently enable types and numbers of analyses which would otherwise be impractical, they can also be costly and time consuming. It is therefore essential that planners give careful attention to insuring that their use is cost-effective.

The model evaluation and selection procedures described here are specifically oriented to water quality and water resources planners and managers. They are designed to enable a planner without previous experience in water quality modeling to determine whether a receiving water quality model could and should be used in a particular planning program, and which specific model would be most cost-effective.

The two primary purposes of this work were to develop a technique which would assist planners in selecting and using water quality analysis methods which are cost-effectively matched to their planning responsibilities, and to summarize the technique into handbook form. The handbook is designed to provide planners with a sufficient introduction to water quality modeling to enable effective communication with systems analysts and administrators regarding water quality modeling. Besides model selection and evaluation the handbook[1] also provides guidance on the management of modeling and the use of contractual services.

Method

A systematic way of evaluating water quality models was sought. Clearly, the evaluation procedure would require answers to many specific questions about the models and so a tabular format for presenting these questions and answers was clearly preferred. Tables represent the condensation of large quantities of descriptive text, enable far more rapid information retrieval, and greatly facilitate the comparison of different models. This tabular method of evaluation was used directly in the procedures developed for both model cost-effectiveness analysis and for final model selection.

Information on the models may be obtained from program documentation and user's manuals, published articles about model development and applications, and if necessary by direct communication with the developers and users. Most available water quality models can be located at the following institutions: the Environmental Protection Agency, the Army Corps of Engineers, the U.S. Geological Survey, state water quality planning offices, and colleges and universities active in the water quality area. The models chosen to develop and demonstrate this technique are all useful for the prediction of water quality and provide a wide range of capability and applicability. At the time (1974-75), they seemed to represent a large portion of the models expected to be in use in the near future. This does not imply that another model, not initially included, might not be preferable in a particular case. The primary function of the selected models was to provide a vehicle for development and demonstration, rather than to draw any conclusions about them. The chosen models for these demonstration purposes are all deterministic simulation models of varying complexity. They were arranged into the following six groups, in accordance with their areas of applicability:

Group I	Steady-state Stream Models
Group II	Steady-state Estuary Models
Group III	Quasi-dynamic Stream Models
Group IV	Dynamic Estuary and Stream Models
Group V	Dynamic Lake Models
Group VI	Near-field Models

The models used to simulate only stream conditions are least complex due to the one-dimensional characteristics of flow. Models for simulating stratified lakes and reservoirs fall next in line of complexity, followed by estuarine models. Estuary models are more complex because the prototype flow is usually in at least two dimensions, and the boundary conditions, such as tides, vary rapidly compared with those in lakes. The costs of model application tend to be proportional to their complexity.

The "quasi-dynamic" model category (Group III) have been so named since only their weather (meteorological) inputs may be dynamic. Their solutions have steady-state hydraulics, but dynamic water quality. The near-field category (Group VI), is the only one in which very localized effects, such as plume entrainment, are simulated.

There exist many other models different from the models chosen for this development and demonstration, as well as other versions of those employed here. A number of these were treated in a similar but less extensive manner in an earlier study by the authors.[2] Probably much the same questions would be used in the evaluation of other models, and only different answers would be obtained in some areas.

Types of models notably different from those evaluated herein include: ecologic modeling of receiving waters, in which the life forms are of prime interest; truly two-dimensional flow models, in which velocity components are determined in two perpendicular directions over a grid of points covering the water body; three-dimensional models which are still more complex and presently are far from being ready for wide use in planning; "continuous" deterministic models, whose output can be statistically analyzed for probability studies, but which need much longer records of water quality data and far longer computer run times; and stochastic models, which provide an alternative approach to the question of probabilities.

Results

The resulting model evaluation and selection technique divides naturally into two stages; model evaluation, and cost-effectiveness evaluation. The latter depends heavily upon the former.

Model Evaluation

The questions to be answered in the evaluation of the models were organized according to their purposes and contents into the fourteen categories listed in Table 1. For each of these categories, a table was prepared which contained from two to six columns, one for each of the specific questions in the category. Table 2 is an example of such a table, in this case for the thirteenth category of Table 1. In each row of Table 2 the answers are entered for each model chosen for evaluation. These tabulations of answers then provide the information which is used to measure the suitability of the models for a particular purpose (its performance index), and the total cost of operating the models.

Table 1

MODEL EVALUATION CATEGORIES

MODEL CAPABILITIES

- Applicable Situations
- Constituents Modeled
- Model Factors Accounted for

DATA REQUIRED

- For Model Inputs
- Additional, for Calibration and Verification

MODEL COSTS

- Initiation Costs
- Utilization Costs

MODEL ACCURACY

- Representation
- Numerical Accuracy
- Sensitivity to Input Errors

EASE OF APPLICATION

- Sufficiency of Available Documentation
- Output Form and Content
- Updateability of Data Decks
- Modification of Source Decks

Cost-effectiveness Evaluation

A form of cost-effectiveness evaluation was determined to provide the most appropriate basis for model selection. The procedure developed to evaluate the cost-effectiveness of each model requires making a comparison of its performance index (PI; a measure of the model's suitability for a particular purpose) with the total cost of operating it.

Clearly the process of selecting a water quality model for any wastewater management planning project may involve numerous complex considerations. Therefore the procedure had first to identify the important factors which influence the selection of models by planners, and then to structure the consideration of these factors in such a manner that confusion is minimized. Of great importance, the procedure does not tell planners what decisions on models to make; instead it provides them with the essential questions and thought structure upon which they or their assistants can make the decisions.

The model selection process is designed to give users a choice of several different levels of detail they may want to consider. The process is therefore divided into four phases, each going into progressively more detail and requiring progressively more effort. These phases are:

Phase I: Model Applicability Tests

Phase II: Cost Constraint Tests

Phase III: Performance Index Rating - Simplified

Phase IV: Performance Index Rating - Advanced

The rejection of candidate models in one phase reduces the number of models to be evaluated in the next phase, and phases are designed accordingly. All considerations in the selection process are based upon the results of the model evaluations discussed previously.

After having identified the problem and inventoried the data available for a particular planning program, the basic decision must first be made whether any water quality model at all should be used. This decision must take into account whether a model would be helpful in plan formulation and whether a suitable model and sufficient data are available. (Any additional data gathering should be postponed until after the models are selected.) Generally, water quality models are useful in any area where the quantitative relationship between varying wasteloads and resulting water quality must be known. However, in "Effluent Limited" areas, waste treatment alternatives will often be specified by Federal Effluent Standards, thus eliminating the need for a water qaulity model. Where there is some doubt whether water quality modeling is inappropriate or inefficient in a particular planning application, the model selection process will soon make this fact apparent.

A set of candidate models must be identified before the model selection process can be initiated. Although the models chosen for demonstration purposes (see Table 2) could be used as the candidate set, many other models are available which should be considered. The planner should select his set of candidate models using as many sources as possible. Since model titles are frequently descriptive of their capabilities, the planner should first use the titles to screen out those obviously not applicable to his particular problem. For the purposes of model selection, there is obviously no need to complete the extensive (fourteen category) model evaluation

Table 2

MODEL SUMMARY: EASE OF APPLICATION, UPDATEABILITY OF DATA DECKS

MODEL		CARD CHANGES (Column 1)	RECOMPUTATION TIME (Column 2)	HELPFULNESS OF AVAILABLE DOCUMENTATION (Column 3)
I	DOSAG-I	Few.	Very small.	Good.
	SNOSCI	Few.	Very small.	Good.
	Simplified Stream (SSM)	None.	Relatively large.	Good. Needs thorough study and good understanding, before using charts.
II	ES001	Few.	Small.	Good.
	Simplified Estuary (SEM)	None.	Relatively large.	Good. Needs thorough study and good understanding, before using charts.
III	QUAL-I	Very small, except for changes of weather data which may involve many cards.	Small.	Good.
	QUAL-II	"	Small.	Good.
IV	Dynamic Estuary (DEM)	Few in most cases.	Small.	Good.
	Tidal Temperature (TTM)	Small, except for weather inputs.	Small.	Good.
	RECEIV	Small, except for transient waste inputs.	Small.	Poor.
	SRMSCI	"	Small.	Good.
V	Deep Reservoir (DRM)	Small, except for weather data.	Small.	Generally good. The three comprising documents are less convenient to use.
	LAKSCI	Small, except for weather and inflow quality data.	Small.	Good.
VI	Outfall PLUME	Minor changes, of at most a few cards.	Very small.	Adequate.

for models which are rejected by applicability or constraint tests (Phase I or II) of the cost-effectiveness evaluation. Therefore, the model evaluations should be accomplished concurrently with, and only to the extent needed by, the various tests and ratings of the cost-effectiveness phases.

For similar reasons, no model should be processed in a subsequent phse until all aspects of the preceeding phase are complete.

The detailed procedure for selecting a water quality model is discussed in the following subsections, one for each phase. A flowchart guide to the procedure has been prepared for each phase. At the end of any phase the user should decide whether to select a model on the basis of the factors he has considered thus far, or whether to refine his analysis further in the next phase. Worksheets, similar in form to Table 2 but containing columns for the entries indicated in Table 3, are required to record the cost-effectiveness evaluations for each phase worked. The more phases the planner uses, the more confidence he can have in his selection. However, there will be trade-offs between selection effort and selection confidence, and for many applications adequate confidence in the selection will be attained after completing only the first one or two phases of the process.

Applicability Tests (Phase I). These tests ask questions about the appropriateness of the models for the problem at hand, and inappropriate models are rejected from further study. This first phase of the selection process is therefore very important, because of its rapid narrowing down of the field of candidates.

Results of the applicability tests should be recorded as a "yes" or "no" in the appropriate columns of the worksheet; the categories to be tested are given under Phase I of Table 3. As the various tests proceed, rejected ("no") models should be deleted from subsequent worksheets to avoid unneeded further work.

The ability of a model to simulate the behavior of the correct type of water body is of prime importance. The user can usually determine this capability of a model from the general description in the model documentation. For a deeper understanding, the scale of interest and the extent of concentration and/or flow variability should be analyzed. The time variability test determines whether the needed time-varying model variables are provided by the model. The time varying requirements are established by the length of the simulation period, and by the variability of the flow, quality and weather inputs. The discretization test determines whether a model can simulate the level of spatial detail required for the proposed application; special features such as the presence of tidal flats, flow augmentation sources, and storm loadings may influence this requirement. The constituents capability test simply requires comparing the model capability to simulate water quality constituents with the user's needs; some models have specific constituent capabilities, others can be used for whole classes of constituents which have certain types of kinetic reaction, such as first order decay. The driving forces and boundary factors test involves checking that the model is capable of simulating all the important driving forces in the prototype; some of these may need to be time varying boundary inputs. The various tests of

Table 3
SUMMARY OF COST-EFFECTIVENESS EVALUATION TABULATIONS

COST-EFFECTIVENESS EVALUATION CATEGORIES	PHASE I		PHASE II					PHASE III		PHASE IV		PHASE ALL
	Applicable?	Applic. Limitations	Time	Cost/Run	Cost	Time OK?	Cost OK?	Rating	Weight	Rating	Weight	PI Rating
APPLICABLE SITUATIONS												
Water Body	A							R	W			
Time Variability	A							R	W			
Discretization, etc.	A							R	W			
CONSTITUENTS MODELED												
Constituents Modeled	A							R	W			
Driving Forces, Boundary Factors	A							R	W			
DATA REQUIREMENTS FOR MODEL INPUTS												
Hydrologic and Geologic	A	A						R				
Water Quality	A	A						R				
Effluent	A	A						R				
Other	A	A						R				
DATA REQUIREMENTS FOR CALIBRATION AND VERIFICATION												
Hydrologic and Hydrodynamic	A	A						R				
Water Quality	A	A						R				
Overall Data Rating								R	W			
INITIATION COSTS												
Model Acquisition			A		A							
Equipment Requirements			A		A							
Data Acquisition			A		A							
UTILIZATION COSTS												
Machine Costs				A	A							
Manpower Costs			A		A			R	W			
Total Costs			A		A							
Cost Constraint Tests						A	A					
ADVANCED PI RATING												
Internal Factors Accounted For										R	W	
Model Representation Accuracy										R	W	
PI RATING, STAGE 2												
Numerical Accuracy										R	W	
Sufficiency of Available Documentation										R	W	
Output Form and Content										R	W	
Updateability										R	W	
Ease of Modification										R	W	
OVERALL PI RATING												R

A = Answer (yes, no, $, weeks, etc.); R = Rating on scale 0-10; W = Weight, normalized about 1.0.

data requirements are designed to ensure that the quanity and quality of the available prototype data are satisfactory for the needs of the model. While performing these tests, hoever, it is important to consider whether additional data can be specifically acquired during the project, or whether the model will be used over a number of years during which data collection will probably improve. Entries under the "Applicability Limitations" column of Table 3 should be briefly descriptive.

Any models deemed marginally applicable in the Phase I tests may be maintained for further consideration in Phase III, when their level of applicability will be given a rating.

Cost Constraint Tests (Phase II). In this phase of the cost-effectiveness evaluation both elapsed project time and dollar costs are considered as cost items, which must be compared for each model with user constraints. Answers to most of these tests (see Phase III of Table 3) probably will be either in weeks or in dollars, obtained from the preceding model evaluation (similar to Table 2).

Model acquisition costs will frequently be nominal, though delivery time may be a factor, and some may include a surcharge for each run made. Other models may require a lease or purchase agreement. Equipment requirements for calculators and computers with their peripheral equipment must be compared with the available capabilities, although many services are available through remote terminals. Data acquisition costs summarize the costs of acquiring any additional data, as discussed under Phase I. Machine costs include charges for computation plus the use of various peripheral equipment. Computation time is about proportional to the number of constituents modeled, discrete segments modeled, time steps used, and runs made. Manpower costs include considerations of the number of personnel and the level of expertize needed for a model, possible recruitment and/or training time, model set up time, run time, time to analyze the results, and, of course, personnel salaries and overhead costs.

From the above, estimates of the total cost and time requirements for a model can be obtained. In the final cost constraint tests these are compared with the project resource constraints, and grossly unacceptable models rejected. Marginally unacceptable models probably should not be rejected in this phase because of the approximations undoubtedly necessary in making the many cost and time estimates.

Simplified Performance Index Rating (Phase III). This portion of the model selection process gives a method for estimating the effectiveness of the candidate models. The effectiveness is obtained through a "Performance Index Rating", which is divided into two parts. The first, "simplified" part (Phase III) accounts for the more basic, and usually more important model attributes which have previously been discussed in the Phase I and Phase II tests. The second "advanced part of the Performance Index (PI) rating, performed in Phase IV, involves much more detailed and usually somewhat less important considerations of the models. In most cases, Phase III will give the planner a very good idea of which model is best for his particular planning problem. A brief review of the contents of the second part (Phase IV) will then usually indicate whether those further considerations are necessary.

The same categories of model attributes treated in Phase I are now rated more quantitatively, if they have not been previously rejected. This is shown in Table 3; each category now requires a "rating" and many require a "weight" for Phase III.

The user must select attribute ratings based upon his knowledge of the model capabilities and the application needs for the category considered. The rating should fall on the following scale from zero to ten: 10 is excellent, 8 - good, 6 - fair, 4 - poor, 2 - very poor, and 0 - completely inadequate.

The "weights" are used to adjust the impact of each attribute rating on the overall Performance Index, based upon their relative importance. For example, if the "Time Variability" capability of a model is much more important than the "Constituents Modeled" capability, then it should have a larger weight. Weights must be assigned by the planner based upon his judgement of the importance of each attribute to his planning problem. In assigning weights the most significant factor is the relative importance of the various attributes. Therefore they are normalized about a value of 1.0; typical weight ranges are given in Ref. 1. For a particular application a single set of weights should be used for all candidate models. But they will probably vary with each application to a different prototype situation. The user will probably find it more convenient to assign the ratings and weights at the same time as he performs the Phase I tests.

When all Phase III ratings required in Table 3 are complete, the planner should decide whether or not to proceed with more detailed ratings in Phase IV. If the Phase III ratings are deemed adequate for model selection, then the overall performance index of the j^{th} model can be computed using the equation:

$$PI(j) = \frac{\sum_{i=1}^{n} [\text{Rating } (i,j)]\ [\text{Weight } (i)]}{\sum_{i=1}^{n} \text{Weight } (i)}$$

where i = the attribute numbers
n = number of attributes considered

Advanced Performance Index Rating (Phase IV). This final phase enables far more intensive probing into details of various candidate models. Most of the ratings in this phase follow the procedures of Phase III but require extensive user insight and experience in water quality analysis and modeling. For this reason it is included as optional in the overall selection process, and it is not discussed in detail here. The evaluation categories for Phase IV are listed in Table 3, and an overall PI rating for both Phases III and IV could be obtained in the same manner; full details are given in Reference 1.

Final model selection simply requires making a tabulation of the total dollar costs (Phase II) and the overall PI ratings for each model. Table 4 is the result of an example application. The user can make his selection by either comparing costs and expected performance, or by using the PI/cost ratio.

Table 4

COST EFFECTIVENESS COMPARISON

Model	PI Rating (From Phases III & IV)	Total Cost of Application (From Phase II)	$PI*10^4$ / Dollar	Rank
A	6.0	$ 50,740	1.18	3
B	6.1	56,040	1.09	4
C	6.9	53,650	1.28	2
D	7.1	52,740	1.36	1

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Acknowledgements

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A LANDSCAPE PLANNING MODEL AS AN AID TO DECISION-MAKING FOR COMMUNITY GROWTH AND MANAGEMENT

J. Gy. Fabos
Department of Landscape Architecture
and Regional Planning
University of Massachusetts
Amherst, Massachusetts

S. A. Joyner, Jr.
Department of Civil Engineering
University of Massachusetts
Amherst, Massachusetts

Abstract

A landscape planning model for assessing special resources, hazards and development suitabilities is described. Computer mapping aids in the quantitative and spatial mapping of resultant assessments. A framework for incorporating economic evaluations of resources, hazards and development suitabilities into land use decisions is proposed. Application of the model to a town in the Boston Metropolitan Area showing the results of 20 years of Metropolitanization is illustrated.

Background

An interdisciplinary landscape research team was established at the University of Massachusetts in 1971. Since that time, over 30 people have contributed to the development of a Metropolitan Landscape Planning Model (acronym, METLAND). The team has responded to the perceived problem that the "metropolitanization" of eastern Massachusetts has caused a needlessly high depletion of its environmental/landscape resources, has increased hazards, and development has often occurred on marginally suitable lands. Furthermore, metropolitanization has impaired the vital ecological stability of large landscape units. If these phenomena could be quantified, it was argued, an important step would be taken to placing them on equal footing with other quantified "values" and thereby integrating them into the decision making process.[1]

It is well recognized that highways and other major public installations have been the major growth generators; their planners have seldom taken into account the factors described above. The model presented here is designed to provide a procedure to assess special resource, hazard and development suitability potentials, which could complement and benefit existing decision making. The model presented here has been applied to the town of Burlington in the larger Boston Metropolitan region. The Boston metropolis has gradually engulfed 2500 square miles (see Figure 1). Application of the model demonstrates the consequences of this metropolitanization on the town of Burlington. Approximately eighty percent of this town has been developed with modern industries, shopping centers and low density housing.

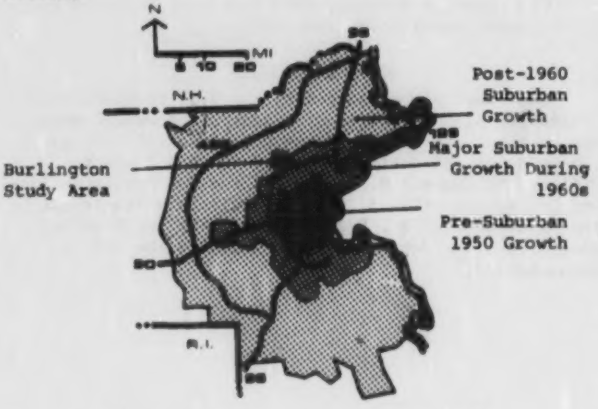


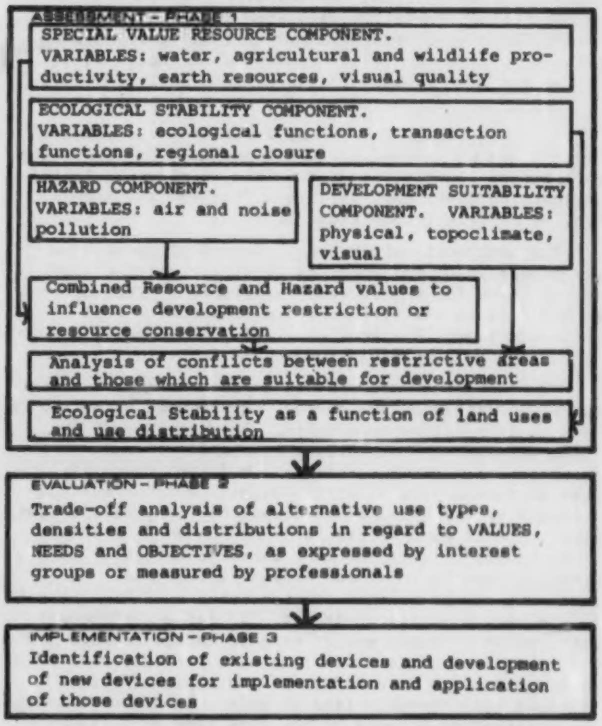
Figure 1. Boston Metropolitan Area[2]

The rationale of the METLAND team has been that the attention of decision makers could be better and more easily brought to focus on these landscape issues if the magnitude of the negative effects resulting from their actions were clearly pointed out. Our research to date has demonstrated an attempt to place economic values on several resource variables. The continuation of this research, however, will investigate other evaluations based on energy use analysis and the perception of various interest groups such as conservationists and developers.

Framework of the METLAND Model

To deal quantitatively with environmental issues of the "metropolitanized" landscape, the METLAND study has proposed a three-phase planning model including assessment, evaluation and implementation phases (see Figure 2). The assessment phase, which is the focus of this paper, will be outlined in detail below. The remaining two phases are in the early stage of development at the time of this writing.

Figure 2. METLAND Conceptual Model



ASSESSMENT - PHASE 1

SPECIAL VALUE RESOURCE COMPONENT. VARIABLES: water, agricultural and wildlife productivity, earth resources, visual quality

ECOLOGICAL STABILITY COMPONENT. VARIABLES: ecological functions, transaction functions, regional closure

HAZARD COMPONENT. VARIABLES: air and noise pollution

DEVELOPMENT SUITABILITY COMPONENT. VARIABLES: physical, topoclimate, visual

Combined Resource and Hazard values to influence development restriction or resource conservation

Analysis of conflicts between restrictive areas and those which are suitable for development

Ecological Stability as a function of land uses and use distribution

EVALUATION - PHASE 2

Trade-off analysis of alternative use types, densities and distributions in regard to VALUES, NEEDS and OBJECTIVES, as expressed by interest groups or measured by professionals

IMPLEMENTATION - PHASE 3

Identification of existing devices and development of new devices for implementation and application of those devices

The assessment phase consists of a selection of variables analyzing the intrinsic value of those environmental characteristics which may produce benefits or result in harm to society. These several resource and hazard analyses are mapped and organized into four groups, called components. While each individual variable has a specific value, this grouping helps to identify complementary relationships and environmental issues and to provide combined values which are useful in making decisions. The four components of the assessment phase are referred to as: (1) special resources, (2) hazards, (3) development suitability, and (4) ecological stability.

METLAND Assessment Components
(Refer to Figure 2)

The special resource component of the assessment phase addresses the issue of environmental resources and specifically deals with three types of resources. These are: (1) renewable physical resources (e.g., water), (2) non-renewable physical resources (e.g., sand and gravel), and (3) "aesthetic-cultural" resources (e.g., views). Both renewable and non-renewable physical resources are critical to the metropolitan region. Aesthetic-cultural resources, while not critical, are nonetheless important because their presence enhances the quality of life. Presently comprising the special resource component are five individual special resources or "variables." Representing the first type of environmental resource are the variables known as agricultural productivity, wildlife productivity (including openland, woodland, and wetland wildlife subvariables), and water resources (including water quality and water supply subvariables). Representing the second type of resource is, at the present time, only the variable of sand and gravel supply. Representing the third resource type is visual landscape quality, which refers to such special landscape features as quality wetland areas, views and historical sites, and the visual contrast, diversity and compatibility of land uses.

The assessment of this component is based on the premise that if a portion of a landscape possesses a high quality and quantity of one or more of these resources, those areas should receive special planning consideration and various degrees of protection from development. If immediate need for the resources is not apparent, they should be protected or conserved much as capital resources are saved in a bank until they are needed.

Assessment procedures have been developed for each of the special resource variables and subvariables. In addition, a composite resource assessment procedure has been developed to evaluate all special resources together. Although such a composite assessment can be based on any one of several resource value sets, as it was mentioned earlier, METLAND has to date used only an economic evaluation of relative resource significance in compositing individual special resource assessments. (This is also the case in the composite assessments made for other METLAND model components.)

The hazard component of the assessment phase focuses on the issue of environmental dangers or undesirabilities. Presently comprising the hazard component are three environmental variables: air pollution, noise pollution and flooding. The individual assessment of these three hazard component variables provides spatial information on both the type and the magnitude of hazards. The composite assessment of hazards combines this information.

The development suitability component addresses the issue of environmental opportunities for alternative types of development. These opportunities are landscape resources which can minimize the cost of development while increasing human comfort and user amenities. Included in the component are three variables--a physical variable, a topoclimate variable and a visual variable--which enhance the suitability and the attractiveness of an area for development. To date only the physical variable is operational.

The ecological stability component, which is being developed, will deal with the issue of ecological impact, ecosystem structure and function, and the implications of such structures and functions in land use decisions.

The variables and subvariables comprising these four assessment components are the elements designed to perform the specific analyses required for application of the assessment phase of the model. They are also the elements which provide the basic assessment procedures.

METLAND Assessment Procedure and Application

The essential element of the METLAND assessment procedure is a mapped depiction, at a common scale, of the results of the variable assessment. A map, therefore, is prepared for each subvariable and variable. These variable assessment maps are then overlaid to form composite special resource, hazard or development suitability maps for the study area.

With the expansion of the assessment phase of the METLAND model to include special resources, environmental hazards, opportunities for development, and ecological stability, the need for a tool to rapidly digest and manipulate large amounts of data collected on the regional scale, and to prepare these individual and composite variable assessment maps, became imperative. On the basis of a study undertaken to select such a tool, the Computer Mapping for Land Use Planning (COMLUP) system (developed by Dr. Neil Allen of the U.S.D.A. Forest Service) was chosen as most appropriate for the METLAND study.[3] This selection by METLAND of a computerized mapping system reflected the fact that computerized data banks are today becoming available for use by metropolitan regions and communities. It was assumed that this availability would continue to increase in the near future. Below, the capabilities of the COMLUP mapping system are summarized.

The COMLUP Mapping System

The COMLUP system is essentially a computer mapping package of some twenty-five programs with provision for inventory, overlay (including weighting), and line plotting of spatially located source data.[4] For the purposes of the METLAND study, its function has been expanded, by METLAND computer specialist Dorothy Grannis, to that of a landscape planning tool. As such, it not only provides an inventory of existing environmental values and combinations of values, but is also able to estimate or simulate the cause-effect relationship of proposed alternative environmental land use patterns and decisions.

Capabilities of COMLUP

COMLUP is a second generation grid system which followed the first generation or manually applied overlaying of grids, most often referred to as SYMAP.[5] But because remote sensing and other land use survey information is becoming available at a finer scale, a more accurate data storing and manipulating system was needed. The advantage of the second generation COMLUP computer geographic technique over the earlier technology is that any shape and size polygon can be directly input and stored in the computer, by image digitizer, without subdividing the polygon into grid cells.[6] For data manipulation, the digitized area still must be subdivided into cells, but this is now done in a second step by the computer automatically, instead of as a manual first step.[7]

Application of the COMLUP system can be described in a simple three step procedure, as follows. In step 1, the COMLUP program takes the digitized data in line segment form and overlays the grid of fine granularity (500 X 1000 cells) on these data. In step 2, maps are overlaid on one another one at a time by the computer. Step 3 re-converts the grid data back to line format so that it may be plotted on a drum or flat-bed plotter.

The plotted output constitutes a mapped depiction of the results of the applied variable assessment procedure.

Composite assessment maps are prepared in a similar way. The source maps in these cases are the already prepared individual variable assessment maps. The assessment maps of variables belonging to a single assessment component are internally overlaid and weighted as desired. The plotted output is a mapped depiction of the composited variable assessments belonging to the component in question.

The rest of this paper briefly summarizes the application of the assessment phase. The assessment procedure at the variable level will be shown only by one example. An overall assessment is also shown which is produced by the combination of the first three components (special resource, hazard and suitability) shown in Figure 2. The final portion of the paper will summarize the conceptual framework of the evaluation and implementation phases.

Application of METLAND Assessment Phase

In Figure 2, there is an implied difference among the various components. Special resource and hazard components are developed so that development restriction or resource conservation can be achieved. The third or development suitability component, however, is designed to show opportunities for development, from the point of view of physical and topoclimatic suitability and visual amenity values. To describe an assessment procedure of a variable, the physical development suitability variable is selected for illustration. The combined or component assessment incorporates the results of all variables of each component. In this initial study, variables are weighted by economic evaluation.

Physical Development Suitability Assessment Procedure

Surficial geologists,[8] soil scientists,[9] civil engineers and landscape architects[10,11] have studied for decades aspects of physical development suitability. The significance of this variable can be supported by the findings of these researchers. Our investigation identified six subvariables of significance supported by scientific results and estimated added development costs needed to overcome development constraints, when suitability is less than ideal.[12] These subvariables are as follows in the order of their importance: (1) depth to bedrock, (2) depth to water table, (3) drainage (this often overlaps with water table characteristics), (4) slope, (5) topsoil, and (6) bearing capacity. To assess composite suitability based on these six subvariables a simple four step procedure is used:[13]

Step 1: An interpretation of soil types for each of the six physical factor subvariables.

This interpretation is based on (1) the three-part symbols by which the SCS identifies all soil types, and (2) information provided by the SCS Engineering Technical Guide which identifies the dimensions of physical factors (e.g., 0-2' depth to bedrock).

Step 2: An assignment of estimates of expected added development costs to physical subvariable dimensions interpreted from soil types.

On the basis of METLAND research, it has become possible to directly assign actual dollar estimates representing added development costs. The upper limits of these added development costs per acre (assuming that two houses are built with basements on each acre) for each subvariable are as follows: depth to bedrock up to $20,000; depth to water table up to $5,000; drainage up to $5,000 (it should be noted that correcting high water table or poor drainage characteristics can be done together at little extra cost); slope up to $1,300 (but development on slopes greater than 15% is prohibitive for the average development); topsoil up to $1,500; and bearing capacity up to $1,500.

Step 3: A determination of the estimated total added development costs for each soil type.

This is accomplished simply by combining the added costs per physical subvariable for each soil type, with the exception of the depth to water table and drainage variables, in which case only the higher cost is counted for both.

Step 4: An aggregation of total added development costs into A-B-C-D classes for physical development suitability (as shown in Table 1 below).

Table 1

A-B-C-D Classes for Physical Development Suitability

Total Added Costs	Aggregation Class
$ 0 - $2000	A
$2001 - $4000	B
$4001 - $9000	C
$9001 +	Undevelopable (or Class D)

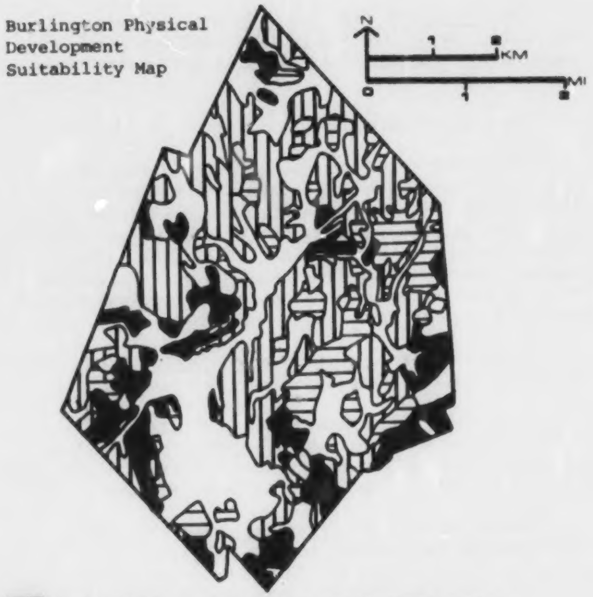
As in each assessment procedure, this type of aggregation serves to categorize soil types in terms of high, moderate and low potential suitability for a typical housing development. In this case, A, B and C classes are based on what total added development costs actually mean in terms of housing square footage. Also in this case, a fourth category referred to as "undevelopable" (or Class D) is considered. The inclusion of this fourth category reflects the fact that there is a significant practical difference between sites that have a low development suitability and those that are entirely unsuitable for development.

Once appropriate A, B, C and "undevelopable," or D classes are assigned to each soil type, the COMLUP system is used as before to produce the desired assessment map for physical development suitability. Figure 3 shows the COMLUP map results of this physical development suitability assessment technique as it was applied to the town of Burlington.

Combined Assessment of All Components and a Preliminary Evaluation

At this writing the majority of assessment procedures for the variables have been developed. The five special resource variables listed in Figure 2 were applied to the study town of Burlington, Massachusetts. The composite assessment of all special value resources and a composite assessment of two of the three hazard variables was prepared. Each of the variables was weighted using economic evaluation. The third map used in this combined assessment procedure was the physical development suitability assessment map. Topoclimate and visual suitability assessments were not included since satisfactory economic evaluations have not yet been incorporated into these procedures.

The specific purpose of this combined assessment procedure is to show the consequences of twenty years of suburban development in Burlington with regard to the three components for which assessment procedures have been developed to date. The town of Burlington has undergone large-scale suburbanization over the past two decades which is typical of the growth trends of many metropolitan communities. In the case of Burlington, this growth is undoubtedly a combined result of the town's proximity to Boston and of the large-scale highway construction activity, which has taken place in the town over the last twenty-five years. For the sake of visual clarity at the present scale, a simplified version of these combined overlays is shown. In addition, since original estimates of resource values, hazard



■ "A" quality areas: added development costs from $0 - $2000/acre

▥ "B" quality areas: added development costs from $2001 - $4000/acre

▤ "C" quality areas: added development costs from $4001 - $9000/acre

☐ "D" quality or undevelopable areas: prohibitive added costs ($9000+)

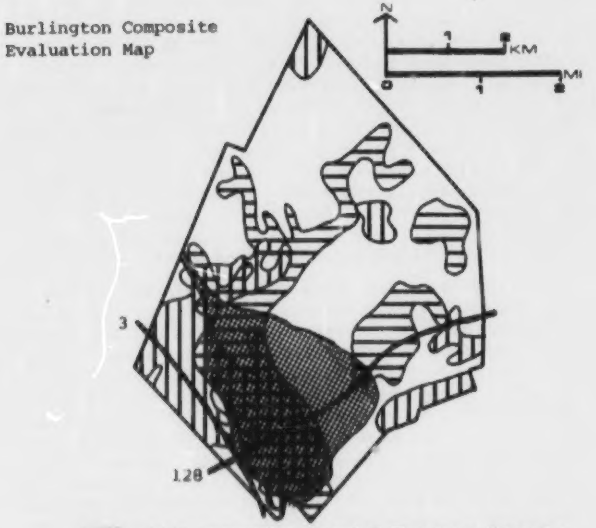
Figure 3. Burlington Physical Development Suitability Map

value losses, and added development costs were based on generalized information unconfirmed by site-specific investigation, combined landscape values are broadly expressed by dollar value ranges. (It should be noted, however, that the COMLUP system can easily compute specific combinations of value and value loss for any desired landscape unit. Also, it should be noted that all economic weightings of values have been substantiated by the team's resource economists. The arguments which support these values are described in the Part II Research Bulletin of the METLAND Research.[14])

The consequences of twenty years of metropolitan suburbanization illustrated in Figure 4 are probably obvious. However, a highlighting of these consequences as they are seen by the METLAND research team is thought to be in order.

First, it should be pointed out that each of the three types of areas identified in Figure 4 indicates the presence of significant land use constraints. These mapped constraints may represent special resource areas which are valuable to people in general, hazard areas which are harmful or undesirable to people and property, or other areas which due to their physical landscape characteristics are especially costly to develop. In Burlington, parcels of land exhibiting one or more of these constraints occupy actually about half the town, or five square miles.

As can be seen, areas having significant land use constraints are concentrated primarily in the southwestern portion of the town. Unfortunately, when one inspects the existing land uses of the town, it becomes evident that post-war land use decisions resulting in land use changes in Burlington were in no way responsive to the presence of these land use constraints. Instead, residential development, particularly single family housing, has been established fairly evenly in all sectors of the town (regardless of the character of the landscape), while major shopping centers and industrial uses have been located almost exclusively along the Burlington stretches of the Route 128 and Route 3 highways.



▤ 1962 Composite Special Resource Assessment Value ($18,000 - $150,000)/acre

▥ 1971 Air and Noise Pollution Hazards Assessment ($1280+/acre damages)

▦ Development Constraint Assessment ($4000/acre added development costs)

Figure 4. Composite evaluation map of special resource values, hazard potentials, and development constraints

These growth-generating highways have themselves been located in that part of the town which has some of the most valuable natural resources together with some of the worst natural conditions for development. As a matter of fact, about two-thirds of the area which is particularly valuable in terms of special resources is also particularly unsuitable for development, requiring average added development costs of as much as $9000 or more per acre to overcome natural constraints for even low density development. These constraints are primarily a result of a very high water table and/or poor load bearing capacity. By glancing again at Figure 4, one is reminded that despite such drawbacks, most of this unsuitable area is not only developed, but is actually developed with massive commercial and industrial structures for which the assessed constraints and compensatory costs are undoubtedly much greater. The irony of this whole land use situation lies in the fact that there is a great deal of land in the town which is distinguished neither for its special resources nor for its natural constraints to development.

Despite these facts, development in Burlington over the past two decades did not follow what appears from all points of view to be the most rational course. There are two principal reasons for this. First, most decision makers during the greater part of the post-war era knew very little about landscape values and constraints as they have been assessed here. Second, even for decision makers who might have known, there were no commonly accepted devices available for implementing protection and conservation planning decisions while satisfying the rights of land owners and developers in an equitable fashion. As a result, land use changes followed and were induced by the location of major transportation routes--a phenomenon which is well-demonstrated here by the Burlington case study.15

Considering the magnitude of the resource loss, hazard increase, and development cost to society proceeding from this pattern of suburban growth, it is firmly believed by the METLAND team that the long-term public interest for planners and decision makers is to take as much account as possible of the natural characteristics of the landscape. Despite the general nature of the results shown in Figure 4, this type of assessment information is absolutely essential to wise landscape planning. At the very least, development decisions should be postponed until estimates of potential landscape value have been confirmed at the site level.

According to the conservative estimates of the team, over 20 million dollars worth of resources were destroyed, hazards increased substantially, and unnecessary development costs soared. The team also developed two alternative growth patterns, one similar to the existing one and another using a P.U.D. type development concept. It was concluded that each growth pattern could easily have accommodated the 25,000 existing population without impairing or loosing landscape resources or exposing so many residents to unhealthy air and noise pollution, or incurring unnecessary construction and site improvement costs. Had either of these plans been adopted originally, the town would today find itself in significantly better shape. Instead of polluted or highly salted local supplies of water, the town would have numerous sources of clean ground water. Instead of having to import sand and gravel from distant sources at ever increasing costs, the town would have accessible local aggregate supplies for development or maintenance projects for many years to come. Instead of being virtually without wetlands and the visual-cultural benefits associated with them, the town would have preserved its major wetland which was filled in to accommodate the sprawling Burlington Mall.

It is realized that economic evaluation has limitations. In broadening the framework of evaluation and developing specific steps for implementation, it is thought important to consider other interpretations based on energy analysis and on the perceptions of various special interest groups (such as conservationists and developers). In addition the team is attempting to propose a procedure which would help an effective participation both of decision makers and of the public in general. These activities are planned to be undertaken in Part III of the research during 1976 and 1977.

While expanding and improving this landscape planning process, the team is convinced that the Burlington case study should provide an impetus for landscape assessment and planning prior to metropolitan invasions. We do not have all the answers, but there is sufficient supporting evidence which shows the utility of this approach.

ENDNOTES

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[2] All graphics prepared by Richard Rosenthal.

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[7] While METLAND is presently using a "second generation" technology, computer programmers are rapidly refining third generation technology designed to overlay polygon areas directly without reconversion to grid cells for manipulation. The Canadian Geographic Information System developed by the Canadian National Government is an example of a completed third generation system (see Ferris and Fabos, 1975).

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A RESOURCE ALLOCATION MODEL FOR THE EVALUATION OF ALTERNATIVES IN SECTION 208 PLANNING CONSIDERING ENVIRONMENTAL, SOCIAL AND ECONOMIC EFFECTS

Douglas Hill
Grumman Ecosystems Corporation
Bethpage, New York

Summary

Modeling for 208 planning should be designed to facilitate participation by planners and representatives of the affected public. Intangibles and incommensurables must be considered, and the ultimate need for value judgments to assess the importance of environmental, social, and economic effects must be accommodated without obscuring the factual analysis. Ideally, population groups that are affected differently should be accounted for separately.

Model building should therefore proceed in successive stages of greater precision. An initial qualitative analysis leads to a conceptual model that identifies the differential impacts of the alternatives, making only the judgment that the impacts are beneficial or detrimental. With land use decisions among the alternatives for satisfying water quality goals, a resource allocation model is useful to account for other costs and benefits. This can be solved for the minimum dollar cost mix of activities as a datum; alternative plans can then be generated by assigning additional importance to intangible and incommensurable values, with the plan selection informed by knowledge of its incremental dollar cost.

Criteria For Modeling in Planning

The nation is embarked on something new in the way of planning making use of models. Under Section 208 of PL 92-500, 150 local agencies are engaged in two-year programs to prepare areawide waste treatment management plans to meet water pollution abatement requirements with "a total resources perspective." In its guidelines for conducting this planning, the EPA(1) emphasizes land use considerations, nonpoint pollution sources, and environmental, social and economic impact evaluation in the comparison of alternatives and selection of a plan.

Almost without exception, the preparation of these plans is in the hands of regional planning agencies, not the departments of public works who have traditionally done water quality planning. As never before, land use planners and water quality engineers are being thrown together to combine their talents. It remains to be seen whether in 208 environmental modeling will provide the organizing structure that focuses interdisciplinary planning or whether it will remain an arcane art practiced by a few professionals.

To the ordinary planner, a mathematical model is a black box which is mysterious if not frightening. If he is trapped in a situation where he must use the results of models, he can no doubt be intimidated into doing so by the authority of his consultants or their peers, but he will be acting as much on faith as if someone were reading entrails. When the contract ends, he will be in no position to judge how his plans should change as conditions change.

Moreover, not only professionals are engaged in 208 planning. The requirement for regular meetings of a citizens' advisory committee seems to be leading to genuine public participation. This may be regarded as a monumental nuisance or as the opportunity to add the dimension that has been missing from most environmental decisions in the past: proper consideration of value judgments.

Environmental decisions necessarily involve both facts and value judgments, and at some philosphical risk, emphasized by Walker(2), a distinction can be made between them.

- o Fact: whether and to what extent as effect occurs
- o Value judgment: whether it is good or bad, and whether that matters

Environmental phenomena described by scientific statements that are subject to test are facts; so are the tangible products of engineering decisions. Whether it is important that certain areas of a bay be safe for swimming is a value judgment. Granted that in the domain of aesthetics where one's very perceptions are determined by one's tastes the distinction may not be clear.

A sequence of analytical steps showing the relationships of facts and values is given in Table 1. The sequence starts with a planned action, shown at the bottom of the diagram, which may have direct environmental, social, or economic effects as indicated by the lower box in each of the respective columns.

The first step in the analysis is to determine whether such an effect occurs (yes/no). If so, the next step is to identify the kind of effect. Identifying the kind of environmental effect may lead to the identification of a social effect (horizontal arrow) not previously identified as a direct social effect. Similarly, identification of the kind of social effect may lead to the identification of an economic impact (horizontal arrow) not previously identified as a direct economic impact.

The next fact that may be determined is the direction of the effect (more/less). On the basis of these facts, a value judgment can be made (horizontal arrows) as to whether the change is beneficial or detrimental to the environment or to man, some of the latter consisting of economic effects. As we illustrate below,

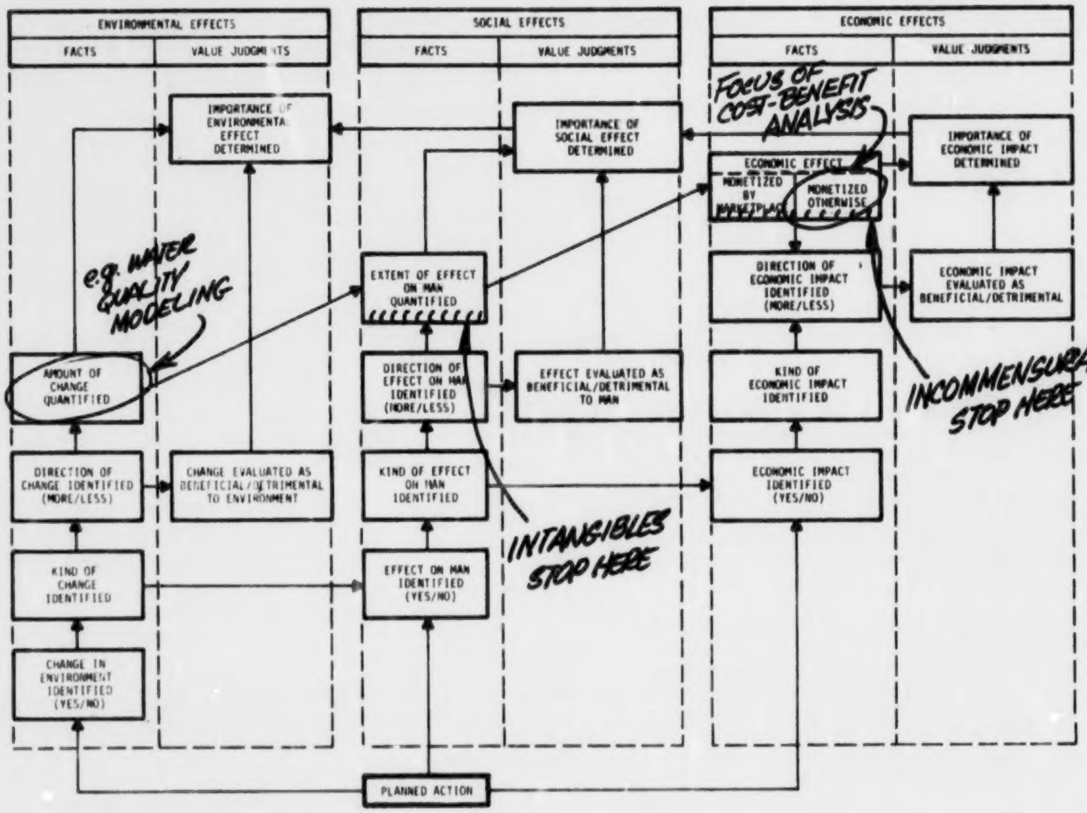

ENVIRONMENTAL EFFECTS
FACTS
VALUE JUDGMENTS
IMPORTANCE OF ENVIRONMENTAL EFFECT DETERMINED
e.g. WATER QUALITY MODELING
AMOUNT OF CHANGE QUANTIFIED
DIRECTION OF CHANGE IDENTIFIED (MORE/LESS)
CHANGE EVALUATED AS BENEFICIAL/DETRIMENTAL TO ENVIRONMENT
KIND OF CHANGE IDENTIFIED
CHANGE IN ENVIRONMENT IDENTIFIED (YES/NO)
SOCIAL EFFECTS
FACTS
VALUE JUDGMENTS
IMPORTANCE OF SOCIAL EFFECT DETERMINED
EXTENT OF EFFECT ON MAN QUANTIFIED
DIRECTION OF EFFECT ON MAN IDENTIFIED (MORE/LESS)
EFFECT EVALUATED AS BENEFICIAL/DETRIMENTAL TO MAN
KIND OF EFFECT ON MAN IDENTIFIED
EFFECT ON MAN IDENTIFIED (YES/NO)
INTANGIBLES STOP HERE
ECONOMIC EFFECTS
FACTS
VALUE JUDGMENTS
FOCUS OF COST-BENEFIT ANALYSIS
ECONOMIC EFFECT
MONETIZED BY MARKETPLACE
MONETIZED OTHERWISE
IMPORTANCE OF ECONOMIC IMPACT DETERMINED
DIRECTION OF ECONOMIC IMPACT IDENTIFIED (MORE/LESS)
ECONOMIC IMPACT EVALUATED AS BENEFICIAL/DETRIMENTAL
KIND OF ECONOMIC IMPACT IDENTIFIED
ECONOMIC IMPACT IDENTIFIED (YES/NO)
INCOMMENSURABLES STOP HERE
PLANNED ACTION

FIG. 1 SEQUENCE OF ANALYTICAL STEPS IN ENVIRONMENTAL MODELING

carrying the analysis only to this point may provide considerable insight into the implications of alternative environmental decisions.

The final step in the sequence of analysis of fact is the quantification of the amount of the change, an example of which is water quality modeling. This may assist in the quantification of social effects on man (diagonal arrow) which may further lead to the monetization of economic effects (diagonal arrow). The monetization of economic effects may be accomplished by the marketplace in terms of market prices. In the case of public goods or bads, however, monetization must be accomplished by other analytical means, i.e., cost-benefit analysis.

Two important classes of effects that cannot be monetized are those that are intangible or incommensurable. Nevertheless, the direction, more or less, of these effects may be determined, and a value judgment made as to whether such an effect is beneficial or detrimental to man. There may be some difference of opinion among individuals as to how aesthetic effects, for example, may become more pleasing; on the other hand, there is likely to be considerable consensus on what is displeasing.

The difficulties in treating aesthetics are great enough that they are usually ignored in environmental analyses, yet we are told by Kneese and Bower(3) that:

> The limited evidence from the studies and analysis...leads to the virtually inescapable conclusion that higher water quality must be justified primarily on aesthetic and recreational grounds, if it is to be justified at all.

Similarly, Ridker(4) observed that psychic costs are likely to be a large portion of the total cost of air pollution. If anything, the aesthetic sensibilities of the public have probably become more acute since these studies were made. In the absence of adequate quantitative methods, assessing the importance of aesthetic effects and psychic costs is largely a matter of judgment.

Between the facts of the matter and their effect on public policy, in short, stands a screen of value judgments. Most properly, these are the concern of the affected public. In environmental studies, they are often ignored or - worse - estimated by technicians as "importance factors." Of the numerous objections to this practice, as Andrews(5) points out, it may in particular obscure the choices to be made by "burying usable information about impacts on specific parameters beneath a layer of questionable value judgments." The expense that may be justified in raising the fidelity of models of the facts in the presence of the noise of value judgments is another question.

In summary, if environmental models for planning are to be improved, they should meet several criteria:

- They should be comprehensible to other planning professionals and the lay public

- They should identify what is important and what is not, preferably early enough to avoid large scale data collection of little relevance
- They should distinguish between facts and value judgments
- They should provide a mechanism that reflects the uncertainty in value judgments and represents the views of the affected public
- They should therefore distinguish sections of the public that are affected in different ways

In attempting to meet these criteria, the modeling procedure proposed here will be described by two examples: (1) a qualitative model to be used near the beginning of the 208 process to determine what is important, and (2) a quantitative model to be used at the end to facilitate making the value judgments needed to select a plan.

Qualitative Model

> To discover profound truths about man and his relations with the world about him, we are well advised to follow two simple rules:
>
> Rule 1. Take a simple idea.
>
> Rule 2. Take it seriously.
>
> Garrett Hardin(6)

The qualitative analysis is based upon the simple idea that a relatively non-controversial judgment can be made as to whether the environmental, social, and economic effects of a planned action are beneficial or detrimental. Taking this idea seriously consists of organizing the results of this analysis and presenting them in a way that clearly illustrates the differential beneficial and detrimental effects of alternative plans on geographical areas or interest groups.

Qualitative analysis is the process of finding how many and what elements or ingredients are present, as in chemistry. The model for planning appropriate to this initial stage of analysis is a conceptual model which although a preliminary and tentative representation of reality should nevertheless consist of the right variables in their correct relationships. A particular value of a model at this stage is its heuristic use as an instrument of discovery to explore the structure of the problem.

As pointed out by Ackoff and Sasieni(7), differences in the degree of obscurity of a problem have produced different patterns of model construction. Inevitably, however, the model builder must decide how to simplify reality in the most satisfactory way. In environmental modeling, this has often led to omitting relevant variables: the intangibles and incommensurables.

In simplifying, the model builder is faced with conflicting objectives: (1) to make the model easy to solve and (2) to make it accurate. At this initial stage, the emphasis should be on making it easy to solve, if possible easy enough for the nonmathematical planner. This can best be accomplished not by dropping variables but by backing off on the requirement for accuracy to only the first step in quantification: whether it is more or less. Moreover, since value judgments provide the final weighting of environmental impacts anyway, the process of "solving" the model at this stage can be short-circuited by the judgment that a given effect will make things better or worse.

This methodology has previously been applied to an environmental analysis of alternatives to dredging a harbor on Long Island, as reported in Wells and Hill(8). Reference will be made to tables originally presented in that paper for illustration.

Procedure for Qualitative Analysis

The procedure for qualitative analysis is as follows:

1. Establish the comparison of alternatives on a valid cost-effectiveness basis, e.g., by comparing the environmental, social, and economic costs of alternatives of equal effectiveness, say, in disposing of equal amounts of wastewater.
2. Determine the geographical areas or interest groups that are affected differentially by the alternatives considered.
3. Identify comprehensively the environmental, social, and economic parameters possibly affected by each alternative.
4. Summarize in tabular form the nature of the impact on each parameter of each alternative.
5. Evaluate whether each of these impacts is beneficial (+) or detrimental (-) to each geographical area or interest group, as illustrated in Table 2, allowing for countervailing effects (±) and uncertainty in the judgment (/). At this stage, this judgment is made regardless of whether the information available is precisely quantitative or merely subjective.
6. Present the pattern of beneficial, detrimental, and countervailing impacts in a matrix of alternatives vs. geographical areas or interest groups. (The summary of all impacts on Port Jefferson, Table 2, is shown as Row 4 of Table 3.)
7. Superimpose on this matrix the identification of the parameters affected beneficially or detrimentally, aggregating those that are affected similarly and noting those that vary identically with an arrow as shown in Table 3.

This final table provides a useful display of the consequences of the choices to be made. It does not make the decision, but it clarifies the decision structure. The beneficial or detrimental implications of the hard scientific and engineering facts are exposed. To choose among the alternatives, further judgments must then be made as to the environmental, social, or economic importance of these consequences, a step best left to the end of the quantitative analysis.

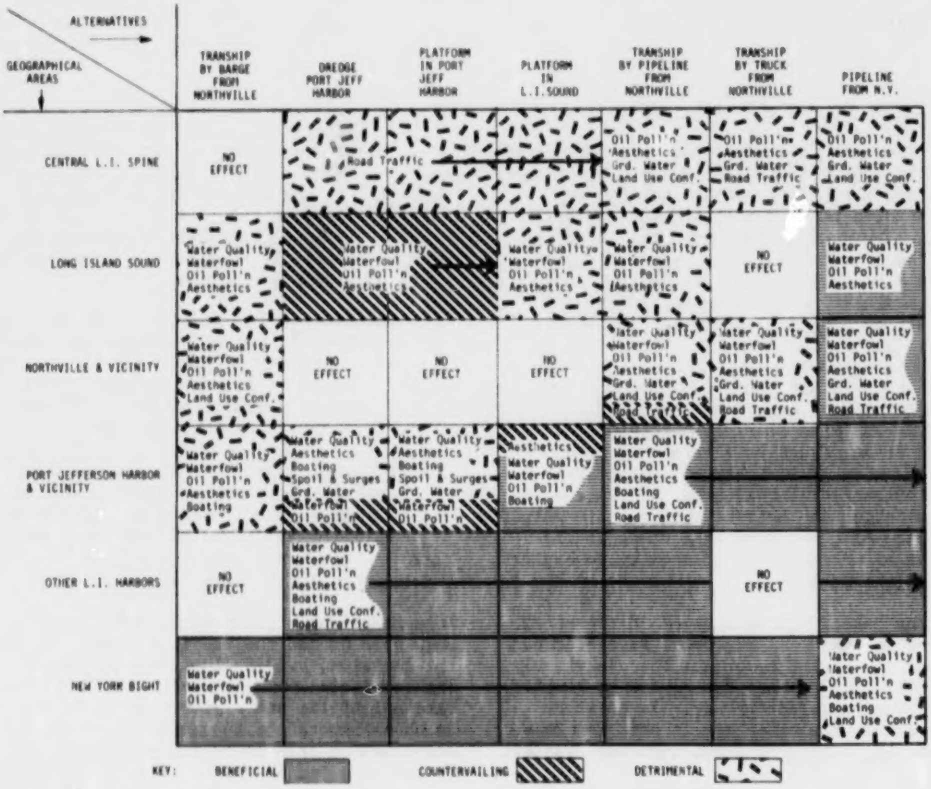
The results of the qualitative analysis consist of the following:

- Geographical areas (and thus population groups) and interest groups affected differentially

TABLE 2 - SUMMARY OF AREA IMPACTS
IMPACT AREA: PORT JEFFERSON HARBOR AND VICINITY

ALTERNATIVES ↓ / PARAMETERS AFFECTED →	Water Quality	Shellfish	Fin Fish	Waterfowl	Other Wildlife	Oil Pollution	Ground Water	Air Quality	Spoil Disposal	Pleasure Boating	Road Traffic	Waves, Surges	Fire Hazard	Aesthetics	Land Use Conflicts	SUMMARY OF ALL IMPACTS ON PT. JEFF
No Modification	←— Baseline Case —→															
Dredge Channel, Basin	0/-	0/-	0	±	0	±	0/-	0	-	-	0	0/-	±	0/-	0	±
Offshore Platform (Harbor)	0/-	0/-	0	±	0	±	0/-	0	-	-	0	0/-	±	-	0	±
(Long Island Sound)	+	+	0	+	0	+	0	0	0	0/+	0	0	+	±	0	±
Transship from Northville: (Truck)	+	+	0	+	0	+	0	+	0	0/+	+	0	+	+	+	+
(Barge)	-	-	0	-	0	-	0	0	0	0/-	0	0	-	-	0	-
(Pipeline)	+	+	0	+	0	+	0	+	0	0/+	+	0	+	+	+	+
Pipeline from New York Harbor	+	+	0	+	0	+	0	+	0	0/+	+	0	+	+	+	+

TABLE 3 - CONCEPTUAL MODEL: ENVIRONMENTAL EFFECTS BY ALTERNATIVE AND AREA



GEOGRAPHICAL AREAS ↓ / ALTERNATIVES →	TRANSHIP BY BARGE FROM NORTHVILLE	DREDGE PORT JEFF HARBOR	PLATFORM IN PORT JEFF HARBOR	PLATFORM IN L.I. SOUND	TRANSHIP BY PIPELINE FROM NORTHVILLE	TRANSHIP BY TRUCK FROM NORTHVILLE	PIPELINE FROM N.Y.
CENTRAL L.I. SPINE	NO EFFECT	Road Traffic →			Oil Poll'n Aesthetics Grd. Water Land Use Conf.	Oil Poll'n Aesthetics Grd. Water Road Traffic	Oil Poll'n Aesthetics Grd. Water Land Use Conf.
LONG ISLAND SOUND	Water Quality Waterfowl Oil Poll'n Aesthetics	Water Quality Waterfowl Oil Poll'n Aesthetics →		Water Quality Waterfowl Oil Poll'n Aesthetics	Water Quality Waterfowl Oil Poll'n Aesthetics	NO EFFECT	Water Quality Waterfowl Oil Poll'n Aesthetics
NORTHVILLE & VICINITY	Water Quality Waterfowl Oil Poll'n Aesthetics Land Use Conf.	NO EFFECT	NO EFFECT	NO EFFECT	Water Quality Waterfowl Oil Poll'n Aesthetics Grd. Water Land Use Conf. Road Traffic	Water Quality Waterfowl Oil Poll'n Aesthetics Grd. Water Land Use Conf. Road Traffic	Water Quality Waterfowl Oil Poll'n Aesthetics Grd. Water Land Use Conf. Road Traffic
PORT JEFFERSON HARBOR & VICINITY	Water Quality Waterfowl Oil Poll'n Aesthetics Boating	Water Quality Aesthetics Boating Spoil & Surges Grd. Water Waterfowl Oil Poll'n	Water Quality Aesthetics Boating Spoil & Surges Grd. Water Waterfowl Oil Poll'n	Aesthetics Water Quality Waterfowl Oil Poll'n Boating	Water Quality Waterfowl Oil Poll'n Aesthetics Boating Land Use Conf. Road Traffic →		→
OTHER L.I. HARBORS	NO EFFECT	Water Quality Waterfowl Oil Poll'n Aesthetics Boating Land Use Conf. Road Traffic →				NO EFFECT	→
NEW YORK BIGHT	Water Quality Waterfowl Oil Poll'n →					→	Water Quality Waterfowl Oil Poll'n Aesthetics Boating Land Use Conf.

KEY: BENEFICIAL ▒ COUNTERVAILING ▨ DETRIMENTAL ⁘

- o Direction of the environmental, social, and economic impacts: beneficial or detrimental
- o Determination of identical impacts among areas
- o Identification of the environmental, social, and economic parameters affected on which data are therefore needed.

For each of the impacts thus identified as discriminating among the subplans and alternatives considered, a further evaluation can then be made as to whether these impacts are:

- Long or short term
- Avoidable or unavoidable
- Reversible or irreversible

Where these distinctions are important in discriminating among alternatives, the information presented in the tabular summaries can be suitably coded. For example, irreversible adverse consequences can be highlighted in the table. We believe that this format is especially suitable to display and discuss the evaluations and methodologies with a nontechnical audience.

This qualitative analysis can be performed very early in the 208 program, since one does not usually begin in a state of complete ignorance of the possibilities. Forcing a preliminary identification of subplans early in the plan development should have the useful effect of focusing the main part of the work on real possibilities. Moreover, the results of this qualitative analysis of the impacts will be available early enough to assure that information needed for the final evaluation is not unknowingly overlooked until the final months of the planning program.

Quantitative Model

The qualitative model identifies the trade-offs to be made; the quantitative model should inform them with data insofar as possible. The purpose of the quantitative model is to define rigorously the information needed to compare subplans, to compile them as mixes into alternative plan packages, and to show the consequences of alternative decisions.

Linear programming models have been used previously to determine efficient degrees of wastewater treatment to achieve specified levels of receiving water quality. With the emphasis on nonpoint sources of pollution, nonstructural water quality controls, and land uses in 208 planning, however, the problem is not simply to minimize dollar costs. Alternative land uses have varying environmental and social as well as economic value, and alternative plans are appropriately cast in the framework of a resource allocation model. On the basis of the qualitative analysis, the resource allocation can be decomposed into geographical areas that can be analyzed as more or less homogeneous units with the local environmental and social impacts of various activities generally judged to be either beneficial or detrimental. An illustration for one such area, a hypothetical estuary in which the use of wetland is at issue, is shown in Table 4. Further details of this model are given in Hill(9).

The use of a linear program to describe in part natural processes which are characteristically nonlinear perhaps deserves some defense. The linear model was used here because it is inexpensive to solve using standard computer software, and because its economic interpretation has been well established. Certainly it will be important to verify that the use of linear coefficients does not do violence to the known facts. The more serious question may be whether enough is known about the natural systems to justify modeling at all, however, not how closely the model simulates reality. Probably the principal value of the model is its identification of the data needed to make an informed decision.

The model is formulated with an economic objective function (Row A) using market values and costs to identify as a datum the mix of activities meeting the constraints at minimum monetary cost. While it is not generally possible to define environmental and

TABLE 4. DATA FOR RESOURCE ALLOCATION IN AN ESTUARY

+ Produces
- Consumes

ACTIVITIES	1. Preserve tall S. alt. (000 Acres) (a) No Filter	(b) Filter Waste	2. Preserve other S. (000 Acres) (a) No Filter	(b) Filter Waste	3. Build & Operate Marina (#)	4. Produce and Harvest Clams (Acres)	5. Produce & Harvest Mussels (Acres)	6. Produce & Harvest Sea Worms (Acres)	7. Produce Cod (000 lb)	8. Produce Flounder (000 lb)	9. Raise Oysters (Acres of Rafts)	10. Fill S. alterniflora (000 Acres)	11. Fill S. Patens (000 Acres)	12. Discharge Untreated Waste Water (MGD)	13. Provide #2 Treatment (MGD)	14. Provide #2 Treatment (MGD)	15. Component Supply	
CONSTRAINTS																		
1. Tall Fringing S. alt. (000 Acres)	-1		0		-0.003	0	0	0	0	0	0	-1	0	0	0	0	+ 0.12	= 0
2. Other Spartina (000 Acres)	0		-1		-0.007	0	0	0	0	0	0	0	-1	0	0	0	+ 1.66	= 0
3. Clam Beds (Acres)	0		0		-0.001	-1	0	0	0	0	0	0	0	0	0	0	+ 50	≥ 0
4. Mussel Beds (Acres)	0		0		-0.002	0	-1	0	0	0	0	0	0	0	0	0	+ 650	≥ 0
5. Sea Worm Bottom (Acres)	0		0		0	0	0	-1	0	0	0	0	0	0	0	0	+ 180	≥ 0
6. Detritus in Bay (000 lb per year)	+4050	+4800	0		+3.6	-300	-240	-2	-1000	-100	-18	0	0	+275	+27.5	+13.8	+ 0	≥ 0
7. Waste Water (MGD)	0		0		+0.005	0	0	0	0	0	0	0	0	+1	+1	+1	+ 0	= 19
8. D.O. Level (mg/l)	-.0146	-.0185	0		-2	0	0	0	0	0	-2.11	0	0	-.052	-.0052	-.0026	+ 15	≥ 6.5 0
9. Nitrogen Load (000 lb per day)	0	-13.1	0	-13.1	+.002	0	0	0	0	0	0	0	0	+.5	+.35	+.05	+ .115 (N) + 3.975 (S)	≤ N
10. Flounders (000 lb)	0		0		-116	0	0	0	0	+1	0	0	0	0	0	0	+ 0	≥ 0
11. Cod (000 lb)	0		0		-400	0	0	0	+1	0	0	0	0	0	0	0	+ 0	≥ 0
12. Fish Ratio	0		0		0	0	0	0	+3.67	-1	0	0	0	0	0	0	+ 0	= 0
13. Marinas (#)	0		0		-1	0	0	0	0	0	0	0	0	0	0	0	+ 0	≥ -1
OBJECTIVE FUNCTIONS																		
A. Annual Net Income ($000)	+35		+35		+133	+6	+1.7	+0.29	+0.207	+0.214	+0.35	+225	+225	0	-56	-87.1		
B. Environmental Value	+		+		±	+	+	+	+	+	+	-	-	-	+	+		
C. Social Value	+		+		+	+	+	+	+	+	+	±	±	-	+	+		

social functions quantitatively, the signs of the coefficients can be judged (Rows B and C). These may be viewed as the direction of corrections that should be made to market prices to allow for nonmarket external effects. Preserving salt marsh (Columns 1 and 2) is estimated to have a market value of only $35 per acre per year, for example, an amount representing rental of hunting rights. This understates the true value of wetlands in their natural state because of their many attributes as a public good: providing habitat and food for fish and wildlife, serving as a nutrient trap for waste water, providing open space that offers aesthetic values, etc. Because of these positive environmental and social values, the amount of $35 per acre per year should be increased in determining the best use of wetland, but it is not known by how much.

The program is therefore exercised parametrically with the value of wetland increasing to determine how environmental and social factors will affect the mix of activities as they are assigned additional importance. For each such change in the program mix, the incremental monetary cost can be determined. This establishes the break-even cost at which one alternative plan gives way to another because of its additional environmental and social value. Part of this incremental cost can be attributed to those benefits that can be quantified. Whether the remainder is sufficient to account for unquantifiable intangibles can be decided with the participation of representatives of the public that will pay the additional dollar cost.

The results of the model are illustrated in Table 5 in which the allocation of wetland is determined in part by their environmental and social value. The minimum monetary cost allocation is described by the bottom row of the table where the market value of wetlands is $35 per year and environmental and social values of wetlands are taken to be zero. Under these circumstances, the allocation of wetlands consists of preserving 120 acres of tall *Spartina alterniflora* and 380 acres of other marsh grass, while 1,300 acres of the other marsh grass is filled for development. If the positive environmental and social values of wetlands are recognized, however, an alternative plan determined by the model consists of the preservation of all marsh grass as shown in the top row of the table. This is determined by the program to have an incremental cost of $247,000 per year which in this case is the opportunity cost of not filling marsh land for commercial purposes.

Thus, the decision makers are presented with the information that if they choose to preserve all wetlands, they are in effect indicating that the community is willing to pay an additional quarter million dollars per year to preserve its environmental and social values. Notice that this result does not state that the environmental and social values of wetland in these circumstances *are* $247,000; it states that the value *must be* worth $247,000 for the decision to be made to preserve all wetlands because of their environmental and social values. Thus it is left to the decision makers to decide on behalf of the community whether this expenditure is justified. Although this kind of result does not give the decision makers the "answer", it narrows the range in which judgment just be exercised.

Environmental decision analysis is largely economic in nature, but it is ultimately political. Models for environmental planning can therefore be no more determinate than the political processes. They will perform a service if they provide the political decision making processes with information on the consequences of alternative decisions. Whether an ordinal comparison that ranks alternatives is sufficient for political decision making or whether a cardinal measure of utility is needed has been a matter of dispute, as debated in Hook(10). Haefele(11) has pointed out that it is the importance of the issue as well as one's preference as to its outcome that makes vote trading possible. Certainly the price that we are willing to pay is a familiar measure of the importance we assign to things as well as the way we reveal our preference. Moreover, recognizing population groups that are impacted differentially, as we have proposed, while not likely to lead to a Pareto optimum in which no one suffers, at least identifies the gainers and losers. The equity with which this trade-off may be made in the larger political context may depend upon the model used for planning.

TABLE 5. WETLAND ALLOCATION vs. ENVIRONMENTAL & SOCIAL VALUE

	WETLAND VALUE		WETLAND ALLOCATION (ACRES)				INCREMENTAL COST
			PRESERVE		FILL		
	MARKET	ENV'L & SOCIAL	TALL S.ALT	OTHER	TALL S.ALT	OTHER	
ALTERNATIVE PLAN	$35	↑ (190)	120	1680	0	0	+$247,000
MINIMUM MONETARY COST	$35	0	120	380	0	1300	——

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REGIONAL RESIDUALS-ENVIRONMENTAL QUALITY MANAGEMENT MODELS: APPLICATIONS TO EPA'S REGIONAL MANAGEMENT PROGRAMS

Walter O. Spofford
Quality of the Environment Program
Resources for the Future
Washington, D.C.

Charles N. Ehler
Office of Air, Land and Water
Office of Research and Development
U.S. Environmental Protection Agency
Washington, D.C.

ABSTRACT

The paper describes the elements of a regional integrated residuals-environmental quality management model developed at Resources for the Future to assist governments in establishing public policy on regional environmental quality--air, water and land--through the explicit analysis of the linkages among gaseous, liquid and solid residuals, and among the various environmental media. Within an optimization framework, the model evaluates a large number of residuals management options including non-treatment alternatives, so that least-cost ways of achieving various levels of ambient environmental quality, subject to constraints on the geographic distribution of costs of achieving these levels, can be identified. The overall management model is made up of three parts: a linear programming model of regional residuals generation and discharge, environmental models (air dispersion and aquatic ecosystem models), and an environmental evaluation section. A summary of results from a test application of the model in the Lower Delaware Valley is presented.

Lessons learned from the development of the Delaware model are related to the objectives and analytic requirements of EPA's current regional management programs, Air Quality Maintenance and Areawide Waste Treatment Management (208) plans.

INTRODUCTION

While it has long been known that the physical environment is an interconnected system, we have traditionally analyzed and regulated it by each of its component media--air, water, and land--ignoring intermedia linkages and possible interform transformations of wastes. The management of wastes, or residuals, from society's production and consumption activities requires decisions regarding environmental quality and economic trade-offs implied in the discharge of residuals into one or more of the environmental media. For example, "clean" air is more likely to result if we choose to discharge residuals to water bodies or place them on the land; "clean" water is highly probable if we choose to discharge residuals to the atmosphere and/or land; and so on. However, if we choose to have high levels of both air and water quality, as well as high quality landfills, then the management decisions become increasingly more complex, requiring information on the physical and economic effects of achieving specified levels of environmental quality simultaneously. The development of this information requires analytical methods that are more sophisticated than those generally in practice today. The purpose of this paper is to discuss regional environmental quality management models in general, and to describe one model, developed over the past four years at Resources for the Future, that potentially has great utility in providing this type of information to decision-makers.

Before discussing the model, however, we will briefly discuss the needs of one possible group of users of this type of model--sub-Federal units of government charged with implementation of two of EPA's regulatory programs, Air Quality Maintenance and Areawide Waste Treatment Management (208) plan development.

EPA'S REGIONAL ENVIRONMENTAL QUALITY MANAGEMENT PROGRAMS

Under the 1970 Clean Air Act Ammendments, in April 1971, EPA promulgated primary and secondary National Ambient Air Quality Standards (NAAQSs) for hydrocarbons, carbon monoxide, nitrogen doxide, sulfur oxides and particulate matter. In addition, standards have been set for photochemical oxidants, even though they are not directly emitted to the air, but are a product of atmospheric reactions between nitrogen oxides and reactive hydrocarbons. National primary ambient air quality standards are specified at a level of air quality necessary to protect the public health. National secondary ambient air quality standards define levels of air quality which are necessary to protect the public welfare from any known or anticipated adverse effects.

After the Federal air quality standards were established, all States were required to submit plans by which they would insure that the standards would be *attained* by 1975. In May 1972 EPA published its approvals and disapprovals of State Implementation Plans (SIPs) and shortly thereafter promulgated substitute regulations for deficient State plans. However, the Natural Resources Defense Council, Inc. (NRDC) and various other petitioners challenged EPA's approvals on several grounds, including the contention that the plans approved were not adequate to ensure *maintenance* of the NAAQSs over time once they were attained. No plan was found that had adequately analyzed the impact of growth on air quality maintenance for any significant period into the future. Subsequently, in March 1973, EPA disapproved all SIPs with respect to maintenance of standards. In June 1973, EPA promulgated regulations requiring States to develop Air Quality Maintenance (AQM) plans for areas with the potential for exceeding a NAAQS between 1975 and 1985. From June 1973 until very recently, EPA and the States have been designating AQM areas. EPA guidelines specified that, at a minimum, the States should consider all Standard Metropolitan Statistical Areas (SMSAs). To date, 168 AQM areas have been designated for at least one airborne residual.

The AQM plan is simply an extension of the SIP. Many of the strategies in the SIP to insure attaineent of the standards can also serve to insure maintenance. Traditional strategies such as the review of new and modified stationary sources and the prevention of their construction if air quality standards will be violated, new source performance standards, and standards for emissions from new motor vehicles might be sufficient to maintain standards in many areas of the country. In most areas, however, these strategies will not be sufficient to maintain standards and it will be necessary to incorporate air quality considerations into the overall context in which decisions regarding metropolitan development are based.

EPA is currently requiring that the plans be submitted as soon as possible for areas that will fail to meet the NAAQSs in the near future; for areas that will not fail to maintain standards until the more distant future, EPA will usually require the AQM plan to be submitted at least 3 to 5 years before measures are actually needed to maintain the standards. While EPA is flexible on the time horizon of the AQM plan, it is encouraging a period of 10 to 20 years as appropriate for most areas. The regulations will require States to reassess, at intervals of not more than 5 years, all areas to determine whether any areas need plan revisions.

Beyond demonstrating that the strategies proposed in the plan are effective in maintaining NAAQSs, the plan must also demonstrate that the State or a substate entity has adequate legal authority to implement the measures contained in the plan. Where measures are included that local governments have traditionally enforced, e.g., minimum thermal insullation requirements for new construction, the AQM plan must demonstrate that a local government has the legal authority to enforce such measures. The plan must also describe the relationships between air quality management and State, local and regional programs for land use, transportation, water quality and solid waste management. Of particular interest are the physical, technological, economic and institutional relationships between AQM and Areawide Waste Treatment Management (208) planning.

The Federal Water Pollution Control Act Ammendments of 1972 (FWPCAA) call for the development of ambient water quality standards "....whenever the State revises or adopts a new standard, ...such revised or new water quality standard shall consist of the designated uses of navigable waters involved and the water quality criteria for such water based upon such uses. Such standards shall be such as to protect the public health or welfare enhance the quality of water, and serve the purposes of the Act." The "purposes" of the Act are defined to include "....an interim goal of (ambient) water quality which provides for the protection and propagation of fish, shellfish, and wildlife and provides for recreation in and on the water be achieved by July 1, 1983."

Section 208 of the FWPCAA calls for Areawide Waste Treatment Management Planning in areas with substantial water quality management problems due to urban-industrial concentrations or other factors. Particular emphasis is being placed in 208 planning on the "software" or implementation aspects of water quality management (e.g., economic incentives, land use management measures, etc.), in addition to the traditional technological options. 208 planning also places particular importance upon the development of management strategies for non-point sources.

To date, 149 areas have been designated as 208 planning areas, but it is anticipated that eventually most SMSAs, approximately 250, will be covered by 208 plans. In addition, all 50 States must prepare plans for non-designated areas of their respective States. Plans must be submitted to EPA two years after the work plan is declared operational, but not later than November 1, 1978. The planning time horizon for 208 planning is 20 years.

Specific plan outputs include the identification of anticipated municipal and industrial treatment works over a 20 year period, identification of urban stormwater management systems, a program for the management of residuals generated in treatment (secondary residuals), and a program for non-point source management. As in Air Quality Maintenance plans, the 208 plan must demonstrate that the strategies proposed are enforceable and must identify agencies authorized to construct, operate and maintain facilities required by the plan, and otherwise implement the plan.

While AQM and 208 plans have slightly different planning requirements, both will perform essentially the same analytical tasks:

1. a survey of existing emissions/effluents, their sources, ambient environmental quality, and an initial assessment of existing and potential problems;
2. a projection of population and economic activities over the planning period;
3. a projection of future emission/effluent discharges, from 2;
4. a projection of future ambient environmental quality, from 3.
5. comparison of results of 4 with standards and a determination of the reduction required;
6. development of alternative strategies to achieve and maintain standards;

and 7. evaluation and selection of a "best" strategy for implementation.

STRUCTURING MANAGEMENT MODELS

Regional residuals-environmental quality management models can be used to analyze the simultaneous impacts on costs and on environmental quality of alternative residuals management strategies. Their basic purpose is to generate information upon which to base public decisions regarding the levels of use and/or protection of the natural environment.

Management models are used primarily to rank sets of strategies according to a given criterion, such as least cost to the region. For this use, the intent is to locate the optimal, or in some sense "best" strategy. In addition, these models are used to explore the range of technologically, economically and politically feasible alternative strategies for the region.

Basically, there are three approaches to seeking an "optimal" strategy for any given objective and set of constraints: 1) response surface sampling using simulation; 2) optimization (mathematical programming) techniques; and 3) a combination of 1) and 2). An example of the latter is exogenous treatment of various levels of low flow augmentation in a water quality optimization model. However, the costs (and damages, if they occur) of providing the various augmented flows are included in the overall ranking of the various management alternatives.

Each approach has its advantages and disadvantages. Simulation models, in general, are able to provide a more realistic representation of real-world conditions, and their outputs are generally easier to obtain than optimization models are to solve. They are conceptually straightforward, and nonlinearities, discontinuous functions, non-steady-state (transient) behavior, and stochastic aspects are much easier to include than with optimization models. However, there are two major disadvantages. First is the general difficulty of selecting *a priori* that combination of raw material inputs, production processes, recycling and by-product production opportunities, and residuals modification activities and levels that optimizes a given objective function. Exhaustive sampling of a finite number of combinations can be used. But because the total number of combinations is usually extremely large, random sampling techniques appear to be a more reasonable approach.

The second major disadvantage with simulation-type management models is the extreme difficulty of exploring the economically and politically feasible range of management strategies, *even when* least cost strategies are not being sought. For regional analyses, economic and political feasibility becomes relevant when it is desired to constrain costs, either the regional aggregate, or the distribution of costs among dischargers, consumers in geographic subregions, and/or among income groups; or the levels of ambient environmental quality at designated locations throughout the region; or both costs and environmental quality simultaneously.

The two major advantages of optimization models are: 1) the direct determination of the activity levels that optimize a given objective function; and 2) the ability to simultaneously satisfy sets of constraints, especially inequality constraints (e.g., upper and lower bounds on activities), and thus the possibility for exploring the range of technologically, economically and politically feasible management strategies. Their major disadvantages, given the magnitude of the regional residuals management problem, are that they are generally difficult to construct and then to solve, even when formulated as linear programming problems. Furthermore, they may not be sufficient representations of the actual (real world) situation. For some cases, a combination of simulation and optimization techniques provides the logical approach to residuals management problems. The use of one technique or the other or a combination would depend upon each individual situation.

There are two basic types of programming models: 1) linear programming (LP) models, and 2) nonlinear programming (NLP) models. Linear programming models are particularly useful when the environmental models (e.g., water quality, air dispersion, and ecosystem models) are formulated as a set of linear relationships. This form of management model is in widespread use today, especially for applications involving the management of regional water quality.[1]

Unfortunately, linear programming models cannot always be used for analyzing regional management strategies, especially if ecosystem models are incorporated within the analytical framework. Ecosystem models are often expressed as a set of nonlinear relationships, and for these situations, nonlinear programming models are necessary.[2]

The regional model and application described in the next section is of this general nonlinear form. The nonlinear programming algorithm used for the analysis is based on the gradient method of nonlinear programming. Unlike the more classical linear management models, the environmental models are not incorporated in the constraint set, but dealt with in the objective function. This modification requires the use of penalty functions for exceeding ambient standards.[3] All nonlinear programming algorithms start from a trial feasible solution and using an iterative search process, select increasingly better solutions until the best possible, or optimal, solution is found. In the application described in the next section, a linear program is used to select better and better solutions. Details of the algorithm and solution procedure may be found in [10,12,13 and 17].

A REGIONAL RESIDUALS-ENVIRONMENTAL QUALITY MANAGEMENT MODEL APPLICATION

In this section we describe the essential elements of a regional integrated residuals management model developed at Resources for the Future by an interdisciplinary team representing the fields of political science, economics, ecology, and engineering.[4] This illustrative application to the eleven-county Lower Delaware Valley region represents the final phase--a real world application--of a research effort at RfF which has concentrated on the development of regional residuals management models to aid government in establishing public policy for regional environmental quality management. Publications describing various stages in the development of the model are available [10-16]. In addition, a fairly detailed description of the regional application, results of analyses using the regional model, policy and research implications, and lessons learned from the application have been prepared [17-19].

The Research Objectives

The major objectives of the RfF research effort and regional application can be stated, briefly, as follows:

1. to investigate the importance of including within a single analytical structure the the linkages among gaseous, liquid, and solid residuals, and the three environmental media;
2. to explore the feasibility of incorporating within a regional optimization model a complex, nonlinear aquatic ecosystem model. An assessment of this objective is not included in this paper, but may be found in [19];

and 3. to explore the ways of designing regional residuals management models to provide distributional information on costs and environmental quality such that these models would be useful in a legislative, as well as executive, setting. The distribution of costs and environmental quality is often the central issue in regional environmental quality management, with efficiency considerations (e.g., least cost strategies) of secondary importance.

The Region

The region that the RfF group selected for their illustrative case study is one of the most densely populated and heavily industrialized in the U.S. The region surrounds the well-studied Delaware Estuary, covers portions of Delaware, Pennsylvania, and New Jersey, and includes the major cities of Philadelphia, Wilmington, Camden and Trenton. For the sake of brevity, let it suffice to note that 5.6 million people resided in the region in 1970. A major concentration of industrial activity spews out enormous quantities of liquid and gaseous residuals to the watercourses and atmosphere in the region, and generates various types and quantities of solid residuals.

The Regional Model

The model, applied to the Lower Delaware Valley region, is designed to provide the minimum cost way of producing 1970 production levels, or "bills of goods," at the individual industrial plans; of meeting electricity, and home and commercial space heating, requirements for the region; of handling, treating, and disposing of specified quantities of municipal wastewater and solid residuals, subject to two sets of exogenously imposed constraints:

1. the distribution of environmental quality--
    - i. in the 22 reaches of the Delaware Estuary: minimum levels of dissolved oxygen and fish biomass, and maximum concentrations of algae;
    - ii. at 57 selected "receptor" locations throughout the region: maximum annual average ground level concentrations of sulfur dioxide and suspended particulates;

iii. at landfill sites throughout the region: restrictions on types of landfill operations which can be employed.

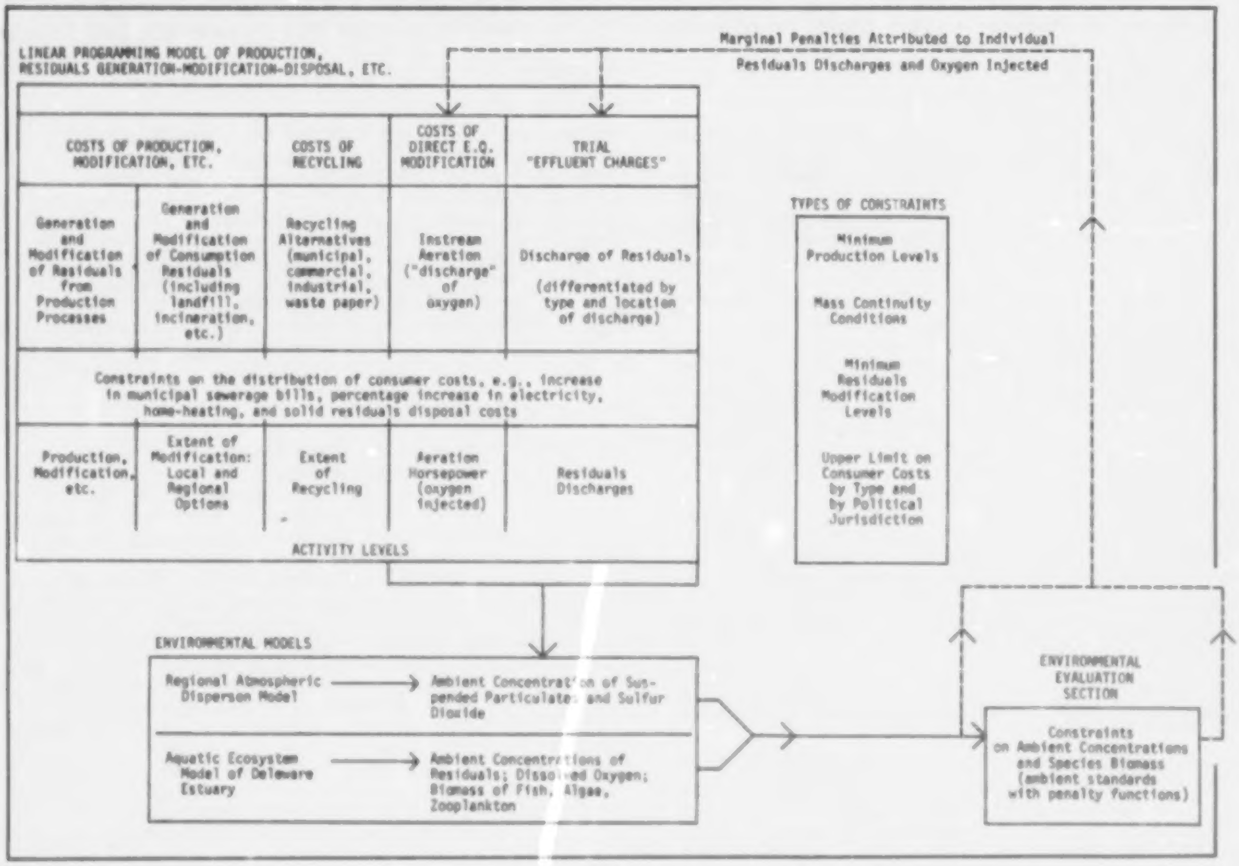
2. the distribution of consumer costs in the 57 political "jurisdictions" of the region[5]--
    i. increases in the costs of electricity (by utility service area) implied by constraints on regional environmental quality (the first constraint set);
    ii. increases in home heating costs implied by constraints on regional environmental quality;
    iii. increases in municipal sewage disposal costs implied by constraints on regional environmental quality;
    iv. increases in municipal solid residuals handling and disposal costs implied by constraints on regional environmental quality.

The regional management model is shown schematically in Figure 1 below. Because the aquatic ecosystem is nonlinear, an iterative nonlinear programming algorithm was employed to search for "optimal" solutions. There are three main parts of the overall regional model: a linear programming model of regional residuals generation and discharge (comprising both production and consumption activities); the environmental models; and an environmental evaluation section. These three major components of the regional model are discussed in more detail below. But first, we should indicate the linkages among these major parts, and the iterative scheme that is used to converge on an "optimal" solution.

A key output of the LP model is a vector of residuals discharges. This vector is input to the environmental models. The output of the environmental models are vectors of ambient environmental quality at designated points in the region. The ambient concentrations implied by a given solution of the LP model are then compared with exogenously imposed environmental "standards." Marginal penalities, based on penalties for exceeding the environmental standards and on the environmental models, are computed and returned to the LP model as prices, or effluent charges, on residuals discharges. This iterative process is continued (in principle) until no better value of the objective function can be obtained.[6]

The LP Regional Activity Model: The LP residuals generation and discharge model describing the major activities in the Lower Delaware Valley region is quite large. It consists of roughly 8,000 columns (variables), over 3,000 rows (constraining relationships), and maintains information on about 800 individual residuals discharges. The following regional activities are included in this model:[7] 7 petroleum refineries, 5 steel mills, 17 thermal electric power plants, 57 home heating activities (one for each political jurisdiction), 57 commercial heating activities (one for each political jurisdiction), 75 large dischargers of gaseous residuals, 36 Deleware Estuary sewage treatment plants, 10 paper plants, 23 municipal

Figure 1: SCHEMATIC DIAGRAM OF THE DELAWARE VALLEY RESIDUALS-ENVIRONMENTAL QUALITY MANAGEMENT MODEL


LINEAR PROGRAMMING MODEL OF PRODUCTION, RESIDUALS GENERATION-MODIFICATION-DISPOSAL, ETC.
Marginal Penalties Attributed to Individual Residuals Discharges and Oxygen Injected
COSTS OF PRODUCTION, MODIFICATION, ETC.
COSTS OF RECYCLING
COSTS OF DIRECT E.Q. MODIFICATION
TRIAL "EFFLUENT CHARGES"
Generation and Modification of Residuals from Production Processes
Generation and Modification of Consumption Residuals (including landfill, incineration, etc.)
Recycling Alternatives (municipal, commercial, industrial, waste paper)
Instream Aeration ("discharge" of oxygen)
Discharge of Residuals (differentiated by type and location of discharge)
Constraints on the distribution of consumer costs, e.g., increase in municipal sewerage bills, percentage increase in electricity, home-heating, and solid residuals disposal costs
Production, Modification, etc.
Extent of Modification: Local and Regional Options
Extent of Recycling
Aeration Horsepower (oxygen injected)
Residuals Discharges
ACTIVITY LEVELS
TYPES OF CONSTRAINTS
Minimum Production Levels
Mass Continuity Conditions
Minimum Residuals Modification Levels
Upper Limit on Consumer Costs by Type and by Political Jurisdiction
ENVIRONMENTAL MODELS
Regional Atmospheric Dispersion Model
Ambient Concentration of Suspended Particulates and Sulfur Dioxide
Aquatic Ecosystem Model of Delaware Estuary
Ambient Concentrations of Residuals; Dissolved Oxygen; Biomass of Fish, Algae, Zooplankton
ENVIRONMENTAL EVALUATION SECTION
Constraints on Ambient Concentrations and Species Biomass (ambient standards with penalty functions)

incinerators, 57 municipal solid residuals handling and disposal activities (one for each political jurisdiction), 23 Deleware Estuary industrial dischargers, and 22 in-stream aeration activities (one for each Estuary reach).

The Environmental Models: Two environmental models are incorporated in the regional model: a nonlinear ecosystem model of the Deleware Estuary [14,15,16] and a linear air dispersion model. The eleven "compartment" ecosystem model, developed at RfF, is based on the trophic level approach. The model was calibrated on conditions that existed in the Estuary in September 1970. Inputs of residuals to the ecosystem model include: organics (BOD), nitrogen, phosphorus, toxics (phenols), suspended solids, and heat. As reported above, target outputs include ambient concentrations of algae, fish, and dissolved oxygen.

The Gaussian plume-type air dispersion model was adapted from the U.S.E.P.A.'s Implementation Planning Program (IPP). Residuals discharges and meteorlogical conditions in 1970 were used to calibrate the model. The model accepts as inputs discharges of sulfur dioxide and particulates, and provides as output ground level, annual average ambient concentrations of sulfur dioxide and suspended particulates.

Model Studies and Results of Analyses

The regional model described briefly above has been run under a number of combinations of air and water quality standards, solid waste disposal restrictions, and assumptions about the availability of two regional residuals management alternatives: in-stream aeration (in the Estuary) and regional sewage treatment plants. For the model runs, the following alternative environmental quality restrictions were imposed:

Ambient Air Quality	Standard Set (E)	Standard Set (T)
SO_2	≤ 120 μgms/m^3	≤ 80 μgms/m^3
TSP	≤ 120 μgms/m^3	≤ 75 μgms/m^3
Ambient Water Quality		
DO	≥ 3.0 mg/ℓ	≥ 5.0 mg/ℓ
Algae	≤ 3.0 mg/ℓ	≤ 2.0 mg/ℓ
Fish	≥ 0.01 mg/ℓ	≥ 0.03 mg/ℓ

Landfill Quality
(3 levels)[a] High(H) Medium(M) Low(L)

Implications for the Lower Delaware Region: For the production runs completed so far, we have found two general implications for the region: 1) the attainment of the national primary air quality standards for sulfur dioxide and suspended particulates will be costly to the region--over $400 million per year (compared with $100 million per year for the less restrictive E level air quality set, and $50 million per year for the most restrictive T level water quality set for the Estuary); and 2) that both the regional management alternatives (in-stream aeration and regional sewage treatment) appear to hold promise for reducing the total regional costs of meeting given ambient quality standards. The total regional costs, and savings due to these regional alternatives, are illustrated in the following table (for T level water quality standards, E level air quality standards, and H level landfills):

Total regional costs ($ million per year)

		In-stream aeration	
		no	yes
Regional treatment plants	no	$190	$155
	yes	$170	$143

Notice that employing both in-stream aeration and regional sewage treatment plants results in a savings to the region of about $47 million per year.

Research Objectives and Lessons: In addition to these general policy implications for the Lower Delaware Valley region, the model results to date have also shed light on the three major objectives of the research with which we started: the inter-media tradeoff question; the use of the nonlinear, aquatic ecosystems models in regional analyses (again, not discussed in this brief paper); and the generation of information on, and the ability to constrain, the distribution of costs as well as physical and biological indicators of environmental quality.

A. Inter-media Linkages: Ample evidence for the importance of linkages and tradeoffs among the qualities of the three environmental media are provided by the results of the analyses, and examples have been provided elsewhere[17,18]. Not enough space exists to repeat all these examples here, but to provide some quantitative evidence of these linkages, the increase in total costs (in $ millions) to the region of improving Estuary quality for specified levels of air quality, given high quality landfills, is shown in the following table:

		Air Quality Standards*	
		0	E
Water Quality Standards*	0	$12.3	$ 96.7
		(Δ = 27.5)	(Δ = 35.4)
	E	$39.8	$132.1
		(Δ = 13.1)	(Δ = 23.0)
	T	$52.9	$155.1

*For definitions of E and T levels of air and water quality, see earlier table; "0" level indicates no ambient standards applied in the analysis.

For the 0 level air quality standards, the increase in total regional cost of moving from the 0 to the E level water quality standards amounts to $27.5 million per year. For the E level air quality standards, this difference amounts to $35.4 million per year. If there had been no inter-media linkages, these differences would have been the same. The difference in total regional costs between the E and T level water quality standards are even more pronounced. For the 0 level air quality standards, the difference amounts to $13.1 million per year; at the E level air quality standards, the difference jumps to $23 million per year.

B. Distributional Information: Distributional information on both environmental quality and certain consumer costs is available as output of the Lower Delaware Valley regional model, and has been presented in detail elsewhere [17]. For the sake of brevity, we will not present this information again here. Rather, we will take this opportunity to discuss the problems we had in trying to obtain certain kinds of distributional information that we desired. In the next section, we will explain in more detail why we think this information would be particularly useful in the preparation of Air Quality Maintenance and Areawide Waste Treatment Management (208) plans.

Distributional information, especially on costs, can be used in two ways, depending on the analysis and on the type of management model employed: 1) it can be used in the unconstrained mode to provide information on the environmental and cost implications of alternative residuals management strategies; and 2) it can be used in the constrained mode to help shape the set of economically and politically feasible residuals management strategies that are selected for consideration. Both programming (optimization) and simulation management models can be used for the former analyses, but only programming models are useful for the latter analyses. Since in most regions the distribution of costs and environmental quality will be a more important issue than regional efficiency, we feel it is important to address the analytical problems associated with attempting to provide information based on *constrained* costs and environmental quality.

We have had relatively little difficulty using the Lower Delaware Valley regional model in constraining levels of regional environmental quality and generating information on the implied costs. And, of course, it would have been still easier, and certainly less expensive, to merely provide information on the implied costs and implied levels of regional environmental quality for various alternative residuals management strategies (however selected). But the real difficulty arose when we attempted to constrain both the levels of regional environmental quality and the distribution of costs simultaneously. There are two primary reasons for this difficulty:

1. when costs and levels of regional environmental quality are constrained simultaneously, infeasible solutions are commonplace (as one would expect *a priori*);
2. the "real world" tradeoffs among distributions of cost, among levels of regional environmental quality and the environmental media, and between levels of environmental quality and costs, are extremely subtle and many, and occur at the very top, and flattest portion, of the regional total cost response surface.

The first difficulty poses a problem for both linear and nonlinear programming formulations. (Simulation models, except in very simple situations, are of very limited use in this type of analysis.) If the run turns out to be infeasible, it may be obvious (from the dual values) which constraints need to be relaxed, but it is not at all obvious by how much these constraints should be relaxed. Clearly, we need much more operational experience here before we perfect this use of the regional model.

Regarding the second difficulty, current nonlinear programming algorithms are simply not practical, especially for the large regional applications, and may not be practical for the smaller (less complex) ones. Most nonlinear programming algorithms become less and less efficient as the optimum is approached. Thus, when the regional efficiency criterion is employed, it makes sense to stop these algorithms short of an optimum. Only modest cost savings (as a percentage of total regional costs) are at stake anyway. But in examining the tradeoffs among the distribution of costs and environmental quality, the important information is not only in the total regional cost dimension, but in a variety of other dimensions as well. It is the range of alternatives (or management strategies) for satisfying broadly stated societal objectives, and of course the resulting implications for individuals' costs and environmental quality, that become of major importance. And here is where the current crop of nonlinear programming algorithms lets us down.[9] Unfortunately, for these very important kinds of regional environmental quality management strategy analyses, our only choice, at this point in time, is to resort to linear programming techniques. And we are currently in the process of restructuring the Lower Delaware Valley regional model as an LP model by removing the nonlinear ecosystem model of the Delaware Estuary and replacing it with the Delaware River Basin Commission's linear dissolved oxygen model.

CONCLUSIONS, ISSUES AND FUTURE RESEARCH

In this paper, we have addressed the use of integrated regional residuals-environmental quality management models in the development of Air Quality Maintenance and Areawide Waste Treatment Management (208) plans. The structure and usefulness of different kinds of regional management models were discussed, and a considerable portion of the paper dealt with an application of such a model to the Lower Delaware Valley region. Admittedly, there are limitations to the use of the RfF model, but the research clearly shed light on two important issues associated with the development of AQM and 208 plan development and strategy evaluations:

1. linkages among the three major forms of residuals and among the three environmental media do exist, and evidence suggests that these linkages are important both in physical and economic terms. Since both of these programs involve significant public investments and imply major effects upon their implementation, to the extent possible, the tradeoffs among residuals and media should be explicitly analyzed;

and 2. ambient environmental quality standards can be met through varying combinations of strategies which can imply substantially different distributions of costs among the public and private sectors, among the residents of the various subregions, and among different income groups. It is clear that at the local level, at least, the distribution of the costs of improving and/or maintaining environmental quality will be the central issue in determining the political feasibility of different strategies, with total regional costs of secondary importance. Thus, to the extent possible, information on cost distributions of each strategy should be generated and presented.

Finally, a model as sophisticated as the Delaware application is beyond the resources of most environmental quality management agencies. However, the insights like those described above can guide research to develop simpler analytic techniques that may be of more immediate application to AQM and 208 planning requirements. An effort to develop a range of techniques in an operational handbook for regional environmental quality management is currently planned at RfF.

NOTES AND REFERENCES

1. Examples of the linear programming formulation for wastewater management purposes can be found in M.J. Sobel, "Water Quality Improvement Programming Problems," *Water Resources Research*, 1 (4), 1965, pp. 477-487; C.S. Revelle, D.P. Loucks, and W.R. Lynn, "Linear Programming Applied to Water Quality Management," *Water Resources Research*, 4 (1), 1968, pp. 1-9; and R.V. Thomann, "Systems Analysis and Water Quality Management," Environmental Science Services Division of Environmental Research and Applications, Inc., New York, 1972.

2. In terms of the complexity involved in incorporating steady-state environmental models within an optimization framework, we find it useful to distinguish among four broad categories: 1) linear relationships where ambient concentrations, R, are expressed as explicit functions or residuals discharges, X, i.e., $R = AX$; 2) linear, implicit functions, i.e., $X = AR$ (note that this equation set can be rearranged by inverting the matrix of coefficients, i.e., $R = A^{-1}X$); 3) nonlinear, explicit functions, $R = f(X)$; and 4) nonlinear, implicit functions, i.e., $X = f(R)$. Classical water quality models fall in the first two categories and aquatic ecosystem models in the last category. For more details, see [13].

3. For the use of penalty functions in nonlinear programming, see A.V. Fiacco and G.P. McCormick, *Nonlinear Programming: Sequential Unconstrained Minimization Techniques* (New York, John Wiley & Sons, Inc., 1968); and/or W.I. Zangwill, *Nonlinear Programming: A Unified Approach* (Englewood Cliffs, N.J., Prentice-Hall, Inc., 1969).

4. The RfF modelling team consisted of Walter O. Spofford, Jr., Clifford S. Russell, Robert A. Kelly, and Edwin T. Haefele with the assistance of Louanne Sawyer, Pathana Thananart, Blair T. Bower, and James W. Sawyer, Jr. Edwin Haefele developed a legislative bargaining and vote-trading model which is not described in this paper. However, the management model reported here is designed to operate in conjunction with Haefele's political model.

5. To provide information on the geographic distribution of environmental quality and consumer costs throughout the region, the Lower Delaware Valley was divided into 57 political jurisdictions of roughly 100,000 people each. To form these jurisdictions, some of the 379 cities, towns, boroughs, and townships that are located in this region were aggregated, and some were subdivided.

6. For details, see [10,12,13, and 17].

7. For details, see Appendix B of reference [17].

8. The three landfill qualities used in the analysis include: low--open dump, but no buring allowed; medium--good quality sanitary landfill; high--good sanitary landfill with shredder, impervious layer to protect groundwater, wastewater treatment of leachate, aesthetic considerations such as fences, trees, etc.

9. Regional environmental quality management models represent only one example of a large set of natural resource allocation problems that would benefit greatly from the development of nonlinear programming algorithms that could deal efficiently with practical, large-scale applications. We hope that these opportunities will one day be recognized by the applied mathematician and operations researchers.

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A COMPUTER MODELING STUDY TO ASSESS THE EFFECTS OF A PROPOSED MARINA ON A COASTAL LAGOON

Kuang-Mei Lo, Ph.D., P.E., Project Manager
Thomas G. King, P.E., Project Engineer
Arthur S. Cooper, P.E., Vice President
of
Connell/Metcalf & Eddy, Coral Gables, Florida

ABSTRACT

A water quality and hydrographic study was conducted to determine the effects of a proposed marina on the water quality of Old Pass Lagoon, located on the northwest coast of Florida.

Utilizing field data, the flushing characteristics of the lagoon were determined using two methods. An estimate of pollutants discharged from engines of boats using the marina was made based on information in the literature. Based on the flushing characteristics and the estimate of pollutants, the post-construction water quality was predicted using a steady state water quality model.

BACKGROUND

The proposed marina at the Sandpiper Cove development is located at the eastern end of Old Pass Lagoon. Old Pass Lagoon is close to Destin and is at the western end of a spit causing the enclosure known as Choctawhatchee Bay. A map showing the location is presented as Figure 1.

As may be seen from Figure 1, Old Pass Lagoon is open at the western end to Choctawhatchee Bay and the Gulf of Mexico.

The mouth is quite narrow - 150 feet at the narrowest point - and this causes considerable bottling-up of the waters of the lagoon. A further bottling effect occurs toward the eastern end of the lagoon where the lagoon narrows to a width of 150 feet at Norreigo Point before widening out in the area where it is proposed that the marina be located.

Tidal motion plays the most important role in water movement and the flushing action in a lagoon. In the Gulf of Mexico the range of tide is uniformly small, but the type of tide varies considerably at different locations. At Pensacola there is usually but one high and one low water each day, while at Galveston the inequality is such that the tide is semi-diurnal when the moon is on the equator and diurnal at times of a maximum north or south declination of the moon. Consequently, in the Gulf of Mexico, the principal variations in the tide are due to the changing declination of the moon.

FIELD SURVEY

A field survey was conducted in order to determine the existing quality of the waters of Old Pass Lagoon. At each of eight stations samples were taken for the measurement of dissolved oxygen, BOD, nitrogen, ammonia orthophosphate. total phosphate, and oil and grease. The analyses were performed at the Connell/Metcalf & Eddy laboratory in Miami, according to procedures in Standard Methods (1). The physical characteristics of the lagoon were determined by measuring nine cross sections.

A dye test was conducted in the proposed marina area in order to determine the longitudinal dispersion coefficient. The dye material used was a solution of 50 grams of Rhodamine-B. The solution was diluted in the field with lagoon water and released at mid-depth. Approximately 150 feet down-current of the point of release, water samples were collected at intervals following the release of the dye. The water samples containing the Rhodamine-B were analyzed with an Aminco-Bowman Spectrophoto-Fluorometer (SPF) capable of detecting and differentiating Rhodamine-B concentrations as low as 5 ppb. The dispersion coefficient was determined to be 4 ft^2/sec based on the solution of the one-dimensional advection and dispersion differential equation (2,3,4).

COMPUTATION OF FLUSHING PERFORMANCE

The flushing performance of the lagoon was computed by two methods. A digital computer model was used to solve the partial differential equations describing longitudinal advection and dispersion by numerical methods and then to compute the reduction in concentration of pollutants due to tidal flushing action. The flushing performance was also computed using the tidal prism theory - a simplistic approach which nonetheless serves as a useful check on the results obtained using the computer model.

Flushing of a tidal water body is primarily controlled by mixing and translation of the tides. When a mass of dye or pollutant is introduced into the lagoon, it is distributed through the water body by the mechanisms of advective and dispersive transport. Advective transport is generally determined by the velocity of the water due to tides and the addition of fresh water. Dis-

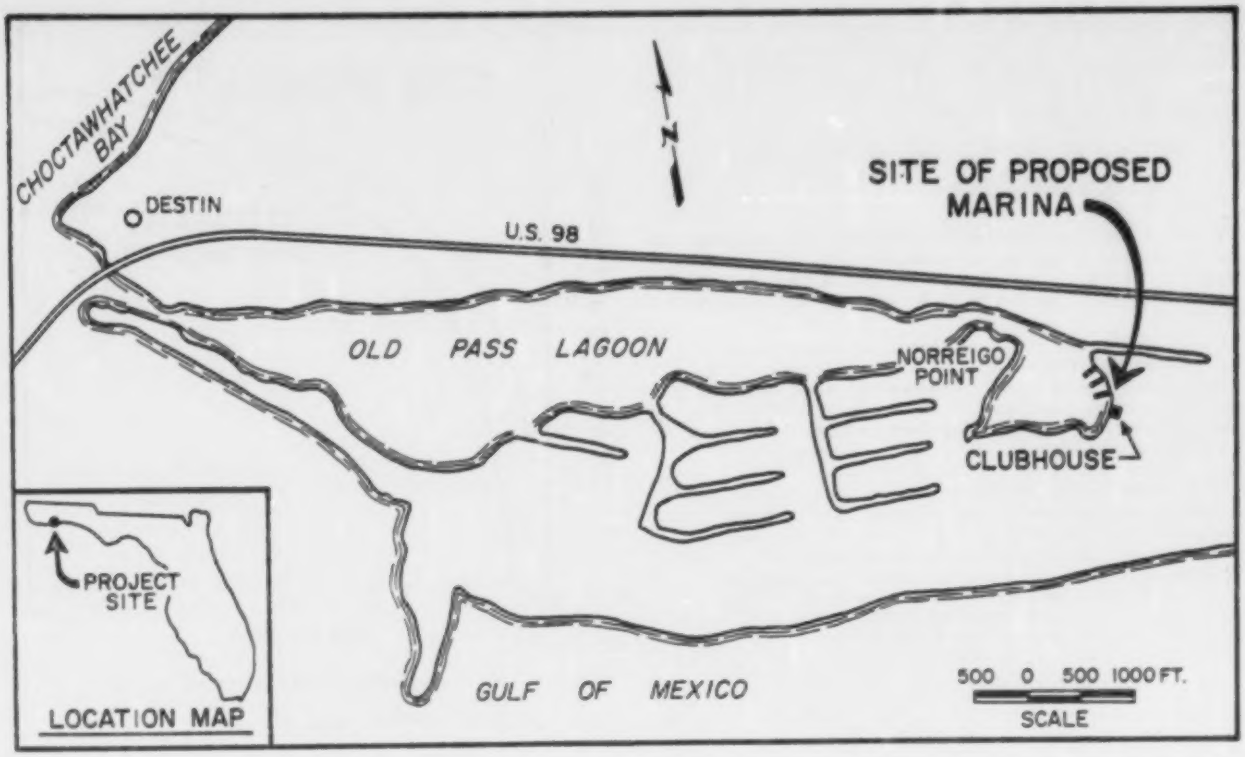

Fig. 1 Map of Old Pass Lagoon Showing the Site of Sandpiper Cove Marina

persive transport is controlled by diffusion which, in turn, is affected by wind, turbulence, and is also considered by many investigators to be a function of the tidal velocity. By assuming that the water is well mixed, vertically and laterally, the flushing of a conservative pollutant can be described by the following partial differential equation:

$$\frac{\partial c}{\partial t} = \frac{1}{A} \cdot \frac{\partial}{\partial x}\left(AD\frac{\partial c}{\partial x}\right) - U \cdot \frac{\partial c}{\partial x} \qquad (1)$$

where:
- c: concentration of the pollutant
- U: mean flow velocity in the cross section
- D: longitudinal dispersion coefficient
- A: cross sectional area
- x: longitudinal distance along the canal
- t: time.

In order to solve this equation by numerical methods, the following initial and boundary conditions are required:

$$c(x,0) = C_0 \qquad c(0,t) = 0 \qquad (2)$$

Thus it is assumed that the initial concentration of lagoon water is C_0 at time t=0, and the concentration at the tidal source is assumed to be zero at all times.

The mean velocity, U, represents the average of the velocities resulting from tidal action and fresh water flow at a given cross section in the lagoon. Since flow due to the addition of fresh water in this instance is minimal, the mean velocity is the average tidal velocity.

To determine this velocity it was assumed that, for a station in the lagoon, the amount of water flowing through the station in a time period Δt was equal to the change in water elevation, ΔH, multiplied by the surface area between the station and the deadend. This relationship can be described by the following equation:

$$AU = \frac{S\Delta H}{\Delta t} \qquad (3)$$

In order to use the above equation to describe the average velocity throughout the lagoon, it is necessary to assume that the tide is uniform with no significant difference in range or phase.

If a mathematical formulation known as the tidal function, H(t), is used to describe the average tidal cycle then Equation (3) may be rewritten.

$$U = \frac{S}{A}\frac{dH(t)}{dt} \qquad (4)$$

The tidal function, H(t), used in this study is chosen from the report entitled "Storm Water Management Model," prepared by the Environmental Protection Agency, October 1971 (5):

$$H(t) = A_1 + A_2\mathrm{Sin}(w) + A_3\mathrm{Sin}(2w) + A_4\mathrm{Sin}(3w) + A_5\mathrm{Cos}(w) + A_6\mathrm{Cos}(2w) + A_7\mathrm{Cos}(3w) \qquad (5)$$

where $w = \frac{2n\pi t}{24}$, n = 1, 2, ... n

and $A_1, A_2, \ldots A_7$ are coefficients.

A computer program employing a least squares procedure was developed to calculate the coefficients in the above equation. Using the computed coefficients, the tidal function for average tidal conditions at Old Pass Lagoon may be written as:

$$\begin{aligned} H(t) = 0.32 &+ 0.084 \operatorname{Sin}(w) + 0.002 \operatorname{Sin}(3w) \\ &+ 0.261 \operatorname{Cos}(w) - 0.003 \operatorname{Cos}(2w) \\ &- 0.003 \operatorname{Cos}(3w) \end{aligned} \tag{6}$$

The cross section information necessary for determining the mean tide velocity was obtained from field measurements and from information presented in Nautical Chart 870-SC published by the U.S. Department of Commerce (6).

To solve Equation (1), the effective longitudinal dispersion coefficient, D, is also required. This coefficient was obtained from the dye test conducted as described above. The value 4 ft^2/sec was used as the average dispersion coefficient throughout the lagoon.

Tidal prism theory was also used to compute the flushing performance of the lagoon. The average turnover rate (or flushing rate) can be computed from the following equation assuming that the concentration, C, of a pollutant in the lagoon is C_0 at time zero, and that the bay is free of the pollutant. The concentration of the pollutant after N tidal cycles is given by:

$$C = C_o\left(\frac{V}{V+\alpha P}\right)^N \tag{7}$$

where: α: mixing coefficent
P: volume of water in tidal prism
V: volume of water in lagoon at low tide.

The volume of water in the lagoon at low tide was calculated from the measured cross sections to be 79,600,000 cubic feet.

An average value for the tidal fluctuation at East Pass Destin was computed to be 0.55 feet from tidal predictions published by the U.S. Department of Commerce (7). By considering this depth of water over the entire area of Old Pass Lagoon, the volume of water entering the lagoon during the rising tide was estimated to be 4,200,000 cubic feet.

It is difficult to accurately assess the degree to which Gulf water is mixed with the lagoon water. It is known that the mixing coefficient is dependent on the tidal and wind velocities as well as the geometric configuration of the lagoon.

An estimate of the mixing coefficient was made by comparing the salinity of Gulf water with that of Old Pass Lagoon. Although no obvious source of freshwater entering Old Pass Lagoon was evident, the salinity in the lagoon was below that in the Gulf of Mexico. By comparison of the salinity in the lagoon before and after the flood tide an estimate of 0.6 was made for the mixing coefficient. With the above information, it is possible to compute the flushing performance of the lagoon using Equation (7).

Since C/C_o is the fraction of conservative pollutant remaining in the lagoon, $(1-C/C_o)$ expressed as a percentage indicates the degree to which flushing has been achieved.

The results of the flushing calculations are presented in Figure 2. They indicate that the time for 50 percent flushing performance is about 30 days for the area in the middle of the lagoon. In other words, this is the time required to reduce the concentration of a conservative material initially distributed uniformly over the canal system to 50 percent of the initial concentration.

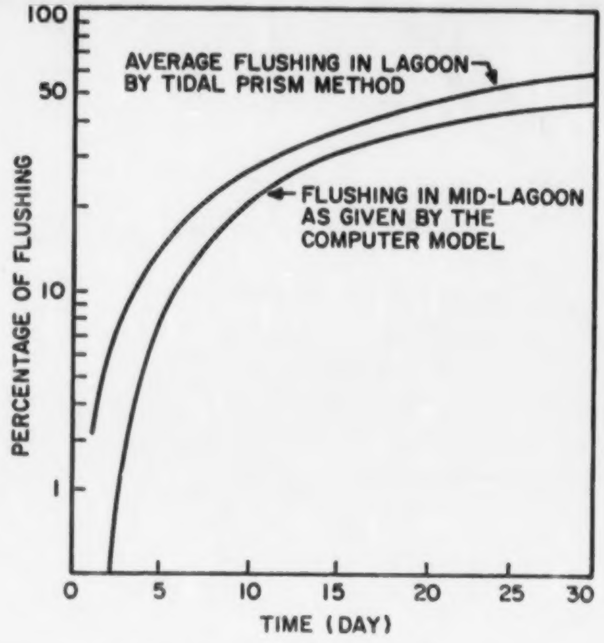

Fig. 2. Computed Flushing Performance of Old Pass Lagoon as Computed by the Tidal Prism Method and the Computer Model

ESTIMATE OF POLLUTANTS FROM THE PROPOSED MARINA

Little data is available regarding the quantities of pollutants that are discharged from the engines of pleasurecraft of the type anticipated to use Sandpiper Cove Marina.

Jackivicz and Kuzminski (8) have presented information on the various compounds found in the exhaust from outboard motors.

The sizes and types of craft expected to use the marina were reported as follows:

Number of Boats	Boat Length	Engine Type
30	20 ft.	Outboard
18	31 ft.	Inboard
14	40 ft.	Inboard

Also, the following conditions are anticipated to be enforced:

- The general public will not be allowed to use the marina.
- An onshore waste disposal system will be available to receive sanitary and other wastes from boats.

Using the information available and making the following assumptions, an estimate was made of the amount of oil that will be deposited in Old Pass Lagoon from outboard engines. The assumptions are:

- Average oil: gasoline ratio - 1:50.
- Discharge of both volatile and nonvolatile oil per boat - 6 gms/liter of fuel comsumed.
- Average usage - twice per week.
- Speed - 15 knots.
- Fuel consumption - 3 nautical miles/gallon.

The distance from the marina to the bridge at the mouth of Old Pass Lagoon is approximately 10,000 feet. Thus, the fuel consumed on two trips in and out of the lagoon may be computed to be 8.32 liters. Consequently, the oil discharged per boat per week is 49.92, say 50 grams and the total oil discharged from the thirty outboard boats is 1500 grams/week.

The biochemical oxygen demand (BOD) and chemical oxygen demand (COD) may also be computed. Under the above assumptions, the time spent per boat operating in Old Pass Lagoon is 26.4 minutes. This may be rounded up to 30 minutes to take into account slower speeds used in the immediate vicinity of the marina. For boats in operation for one hour, the rates at which BOD and COD are generated are 1.05 and 2.50 grams/liter of fuel consumed respectively. Since 8.32 liters of fuel are consumed and there are thirty outboard boats the total weekly demands are 262 and 624 grams respectively.

The above computations have analyzed the effects from outboard engines. Inboard-engined boats do not utilize an oil:gasoline mixture and no data were located that analyze the pollutional aspects of inboard boats. The potential problem from inboard boats centers around discharges from the bilges. However, such discharges are illegal and it must be assumed that stringent enforcement of the law will severely limit such discharges.

For the purposes of this analysis assume that oil is discharged at half the rate as that from an inboard motor, and that BOD and COD are created at the same rates. Thus, the pollutants from 32 inboard boats are:

Oil: 50% x 50 x 32 = 800 grams/week
BOD: 8.75 x 32 = 280 grams/week
COD: 20.80 x 32 = 665 grams/week

The total discharges from all boats at the marina are:

Oil: 2,300 grams/wk = 0.73 lbs/day
BOD: 542 grams/wk = 0.17 lbs/day
COD: 1,290 grams/wk = 0.40 lbs/day

WATER QUALITY MODELING ANALYSES

In order to evaluate the effects of the pollutants generated by boats from the marina, a water quality modeling analysis was conducted using a steady state estuary model developed by Connell/Metcalf & Eddy, Inc. and Hydroscience, Inc.,(9).

The results of the modeling study indicated that the boats using the marina will cause a practically undetectable increase in BOD loading in the lagoon.

Since pollution from oil and grease was the major cause for concern a more detailed analysis of oil and grease pollution was conducted according to the following steps:

(1) The existing oil and grease level in the waters of the lagoon was simulated using a computer model. The results of the simulated oil and grease profile are presented in Table 1.

(2) In order to provide a conservative analysis it was assumed that the oily waste generated by the 62 boats is discharged as a point source at the marina. Initially, the 0.73 lb/day of oil computed above were considered to be generated at the marina. The results of this waste input on the lagoon water are also shown in Table 1. The indication is that the effect on the overall oil/grease level in the lagoon waters is almost undetectable.

(3) Finally, 22 lb/day of oil loading were considered as a point source in the marina area. This figure represents the loading that is applied during a period of 60 days assuming that 50% flushing takes place. It should be noted that this flushing time is much higher than the flushing performance of the lagoon as computed in the previous section and, therefore, the results are conservative.

The above calculation was based on the following assumptions:

TABLE 1. RESULTS OF THE WATER QUALITY MODELING STUDY FOR OLD PASS LAGOON

Location from Hwy. 98 Bridge (ft)	Measured Oil/ Grease Values (mg/l)	Simulated Existing Oil/Grease Condition (mg/l) (1)	Oil/Grease Profile of the Lagoon after inputting 0.73 lb/day Oil/Grease at Proposed Marina (2)	Oil/Grease Profile of the Lagoon after inputting 22 lb/day Oil/Grease at Proposed Marina (3)
600	9.33			
870		7.455	7.484	7.706
1400		6.770	6.804	7.106
1945		6.373	6.409	6.759
2480		6.076	6.114	6.500
2955		5.894	5.943	6.341
3555		5.703	5.744	6.175
4000	3.37			
4215		5.480	5.523	5.981
4825		5.252	5.297	5.783
5220	0.42			
5300		5.085	5.132	5.639
5750		4.878	4.927	5.460
6335		4.640	4.691	5.255
6670	5.81			
7020		4.309	4.363	4.969
7770		3.741	3.802	4.481
8190	0.11			
8270		2.951	3.026	3.806
8570		2.280	2.356	3.222
9195	0.11	1.609	1.159	2.180
9740	0.64			

(1) 4 ft^2/sec was used as the dispersion coefficient. This value was determined from the field dye test conducted near the site of the proposed marina.

(2) It is assumed that the oily waste will be mixed only in the top one foot of water in the lagoon. This is not unreasonable since oil floats but wind and wave action will create mixing.

(3) No freshwater contribution was considered throughout the lagoon.

(4) Oil and grease are considered to be conservative materials. The above modeling analysis indicates that oil and grease discharged from the 62 boats at the marina would result in an increase of the oil/grease content of the lagoon water by about 1 mg/l near the proposed marina site, and about 0.3 mg/l near the outlet of Old Pass Lagoon. The quantity of the increase is considered insufficient to cause deterioration of the lagoon water.

Even though the quantity may not be sufficient to degrade the water quality, oil in such quantity as to be visibly apparent is aesthetically objectionable. Oil films of microscopic thickness are responsible for the bright bands of color that may be observed on the surface of water in canals or on wet roads.

Based on the information contained in a manual on Disposal of Refinery Wastes published by the American Petroleum Institute (10), the amount of oil that will result in a barely visible film on the surface of the water near the proposed marina may be determined.

The American Petroleum Institute reports that an oil film of thickness 0.0000015 inches is barely visible under the most favorable light conditions. Considering the small lagoon area east of Norreigo Point, which has a surface area of 792,000 ft^2, the amount of oil in the film is:

$$\frac{0.0000015}{12} \text{ x } 792000 \text{ x } 7.48$$

$$= 0.74 \text{ gal.} \quad = 6.18 \text{ lb.}$$

Assume that the oily waste discharged into the water due to the marina operations will have disappeared from the surface within 24 hours due to mixing induced by wind, boat traffic and tidal action. Then the 6.18 lbs/day of oil required to maintain a film of oil is over eight times larger than the volume of oil and grease that was estimated to be generated by the 62 boats using the marina.

The assumption that the oily waste will have disappeared from the surface within 24 hours is a conservative estimate. According to the American Petroleum Institute, experiments have indicated that oil films up to 0.0000003 inches in thickness generally do not persist more than 5 hours on an agitated water surface. Tested at sea, less than 24 hours are required to dissipate a film of 0.00004 inches thickness. In general, the thinner the film, less time is required for dispersion.

Furthermore, the 0.73 lb/day oil waste estimated to be generated from the boats will be spread over the entire area of Old Pass Lagoon. In order to be conservative, we have assumed that this waste is discharged near the marina site as a point source.

It should be pointed out that the above calculation is based on the assumption that the oil is evenly distributed on the surface of the water at the vicinity of the proposed marina. It is possible that wind may drive the film to the shore or an inlet and result in a film thick enough as to be visible. There is a tendency for winds to come from the north or from the south, while least wind activity is from the west. This would indicate that there is less likelihood of wind action pushing an oil film toward the deadend of the lagoon and the vicinity of the proposed marina as opposed to driving it out of Old Pass Lagoon.

CONCLUSION

The study indicated that existing water quality in the lagoon is very good. The computations indicate that the lagoon has a relatively poor flushing performance, causing the water to be sensitive to the effects of pollution. However, based on the analysis, it is concluded that the proposed marina and the 62 boats berthed there will have little effect on the water quality of the lagoon.

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DIGITAL COMPUTER SIMULATION OF SECONDARY EFFLUENT DISPOSAL ON LAND

Kuang-Mei Lo, Phd., PE, Project Manager and Connell/Metcalf & Eddy, Inc., Miami, Florida
Donald Dean Adrian, PhD., PE, Professor, Department of Civil Engineering, Uni. of Mass/Amherst

Summary

A computer simulation study was conducted to determine the required field area for an infiltration type of land disposal system based on weather conditions and soil properties. The input information included local evaporation data, average monthly rainfall and average number of days during the month on which it rained, and characteristics of soil's infiltration and drying rates.

The results of this 20-year simulation were used to determine the liquid loading rate under various weather and soil conditions. The liquid loading rate was used to determine the necessary field area for a particular disposal system at a given location.

Introduction

Land disposal of domestic and industrial wastewaters has received a great deal of publicity in recent years. In the Southeast, where climatic conditions are favorable for this type of disposal, widespread interest has been expressed both among professionals in the wastewater management field and the general public.

In general, land disposal is practiced in three ways: spray irrigation, overland flow, and infiltration - percolation. Large land areas are required for all three methods. Over the years, controversy surrounding the long-term effects of the land disposal of effluent, together with the lack of design criteria to determine the land area required, has in many cases forced engineers or planners to disregard this treatment method as a feasible method of disposal. The net result is either failure to consider a viable solution to effluent disposal or creation of additional controversy because many people or groups consider land disposal as the most promising solution for wastewater management.

This paper is primarily concerned with the development of rational design criteria for land disposal, from which an engineer or planner could determine the required land area based on the soil infiltration and drying rates and local climatic conditions. Consideration of chemical and biological changes in the applied wastewater is beyond the scope of this paper. This paper is confined to the study of the Infiltration-Percolation type of land disposal. The best example of this method is the Flushing Meadows Project near Phoenix, Arizona[1].

Description of the System

A hypothetical land disposal system is shown in Figure 1, in which a series of infiltration basins are constructed with soil banks surrounding each basin to prevent entry of surface water runoff. Secondary effluent from a treatment plant is pumped from a storage pond into the basin to a predetermined depth, the basin is kept flooded until a certain amount of effluent has infiltrated, then the basin is dried out prior to the next application. Generally, three major stages are involved in the disposal process. The first stage is called the ponding stage because during this stage effluent is ponded on the surface of the basin and is removed from the basin by infiltration and evaporation. Also, in this period, the volume of the effluent to be disposed of is increased by the rainfall on the surface of the basin. As the disposal process progresses, the second stage is reached when there is no more ponding water in the basin. In this stage, the soil water beneath the basin undergoes a redistribution process which percolates the excessive water from the upper layer to the lower layer of the soil. The rate of redistribution normally decreases rapidly or becomes negligible when the water content in the soil reaches the field capacity. During the re-distribution process, water in the soil is also lost through evaporation. After the soil reaches field capacity, the disposal process progresses to the final stage, drying, during which evaporation proceeds at a rate lower than evaporativity, and the actual rate is dictated by the ability of the soil profile to deliver moisture toward the evaporation zone. The drying process is very important for land disposal because it not only restores the infiltration rates of the soil, it also provides a necessary period for the soil mass to renovate the effluent. During the redistribution and drying periods, the process is also affected greatly by rainfall, which increases the soil water and prolongs the redistribution or drying period. Sometimes when the rainfall is high, ponding water results. Consequently, the process may return to the first stage.

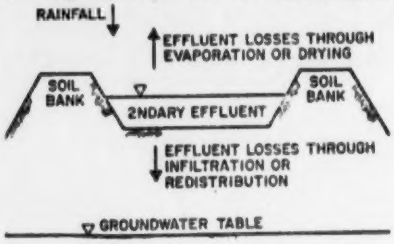
RAINFALL
EFFLUENT LOSSES THROUGH EVAPORATION OR DRYING
SOIL BANK
2NDARY EFFLUENT
SOIL BANK
EFFLUENT LOSSES THROUGH INFILTRATION OR REDISTRIBUTION
GROUNDWATER TABLE

Figure 1. Infiltration Basin

Approach

Because of the stochastic nature of rainfall and its resultant effect on effluent disposal rates, a simulation approach was used in this study to test how a particular design would perform under conditions representative of a given area of the county. To achieve this simulation, mathematical equations to describe the infiltration and drying processes were adopted from the literature to relate soil characteristics to the amount of water lost by infiltration and drying. Input data also included rainfall and evaporation information. Since actual rainfall records are cumbersome to use, synthetic rainfalls were generated for this study. Mean monthly evaporation from a free water surface published by the U.S. Weather Bureau was used to represent water loss to the air during the infiltration and redistribution stages for a given area.

Synthetic Rainfall

A rainfall probability function was utilized to sequentially generate rainfall data using the Monte Carlo Simulation Technique. The generated rainfall data could not be distinguished from historical rainfall data by means of the statistical tests of significance.

The modified Poisson distribution was used by Bagley[2] to represent the frequency distribution of daily rainfall for San Francisco, Sacramento and Spokane. The modified Poisson distribution contains a persistence characteristic so the likelihood of rain occurring on a given day increases if it has rained on the previous day. The Poisson and modified Poisson distribution are compared in Table 1. The modified

Table 1. Comparison of the Poisson and Modified Poisson Distribution

Probability of units of rain (P_i)	Poisson distribution	Modified Poisson Distribution
P_0	$e^{-\lambda}$	$1/(1+d)^{\lambda/d}$
P_1	$\lambda e^{-\lambda/1\,!}$	$\lambda/1!(1+d)^{\lambda/d+1}$
.	.	.
.	.	.
.	.	.
P_i	$e^{-\lambda/i!}$	$\frac{i\lambda\ (\lambda+d)\ldots(\lambda+(i-1)\ d)}{i\ !\ (1+d)^{(\lambda/d+1)}}$

Poisson distribution is a function of two parameters, λ and d, which represents the degree of dependence of one event upon another. When d is zero, the modified Poisson distribution approaches the Poisson distribution as a limit. The procedure by which to calculate λ and d follows an example by Lo[3] which uses Amherst, Massachusetts rainfall records.

From 1961 to 1965 there were 1224 observation days for the interval March to October of each year. In this period, 377 days were considered as having measurable rainfall. The average rainfall in this period was 0.087 inch/day.

If one lets M = total no. of days in the period, N = total no. of days with rain, and U = average daily rainfall for the whole period, then the probability of no rain was (M-N)/M, which must be equal to P_0 as shown in Table 1.

$$(M-N)/M = P_0 = 1/(1+d)^{\lambda/d} \tag{1}$$

or

$$(1225-377)/1225 = 1/\ (1+d)^{\lambda/d} \tag{2}$$

The expected value of the modified Poisson distribution must be equal to U, the average daily rainfall for the entire period. With the unit increment of rainfall of 0.05 inch, the relationship is:

$$\frac{U}{0.05} = \frac{\lambda}{1\ !\ (1+d)^{\lambda/d+1}} + \frac{2\ \lambda\ (\lambda + d)}{2\ !\ (1+d)^{\lambda/d\ +\ 2}} + \cdots + \frac{i\ \lambda\ (\lambda + d)\ .\ .\ .\ .\ (\lambda + (i - 1)\ d)}{i\ !\ (1 + d)^{\lambda/d\ +\ i}} \tag{3}$$

rearranging Equation (1) as

$$\lambda = -[d \log(\ (M - N)\ /\ M\ )\ /\ M\ )]/\ \log\ (1 + d) \tag{4}$$

and solving Equations (3) and (4) simultaneously, we get d = 13.8, and λ = 0.094.

From the probability distribution function, it is then possible to generate synthetic rainfall to represent real-world precipitation. This was done by means of the Monte Carlo simulation technique, in which a subroutine available at the University of Massachusetts Computer Center was used to generate a uniformly distributed random number sequence. Then, by applying a table interpolation method for the inverse probability integral transformation, the random samples of daily rainfall were obtained. Comparison of the generated and recorded rainfall is shown in Figure 2.

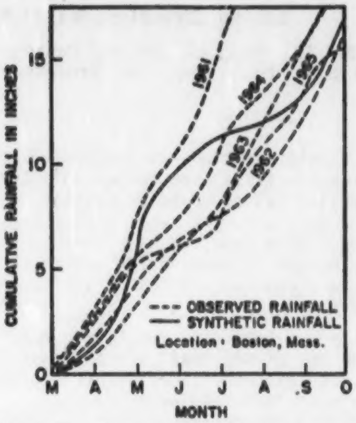

Figure 2. Comparison of the Generated and Recorded Rainfall

Infiltration and Redistribution of Soil Moisture Following Infiltration

Infiltration

Passage of water from a basin to the ground frequently occurs under unsaturated conditions because of the distance between the groundwater table and the ground surface. The movement of water in the unsaturated soil can be described as:

$$\frac{\partial\theta}{\partial t} = - \frac{\partial\theta}{\partial Z}\ (D\ \frac{\partial\theta}{\partial Z}) - \frac{\partial K}{\partial Z} \tag{5}$$

where λ is the volumetric water content, D(λ) is the soil water diffusivity, K is the hydraulic conductivity Z is the distance downward, and t is the time.

Philip[4] developed the above differential equation's solution which describes cumulative infiltration as:

$$I(t) = St^{1/2} + (A_2+K_0)t + A_3\ t^{3/2} + A_4\ t^2 + \cdots \tag{6}$$

Subject to t = 0, Z > 0, $\theta=\theta_1$; and t>0, Z=0, $\theta = \theta_0$

Philip suggested use of the first two terms to describe approximately the infiltration:

$$I(t) = St^{1/2} + At \tag{7}$$

For a larger t, Hillel[5] stated that the cumulative infiltration can be expressed as:

$$I = St^{1/2} + Kt \tag{8}$$

which yields the infiltration rate as:

$$i = \frac{1}{2}\ S\ t^{-1/2} + K \tag{9}$$

where K is the hydraulic conductivity of the soil's upper layer. S was defined by Philip as sorptivity; it can be determined in the laboratory.

Equation (9) describes the infiltration rate of the soil for this study. The infiltration rates used in this study are shown in Figure 3. The rates describe a loamy soil.

Redistribution

The infiltration process then comes to an end when the applied effluent is depleted by evaporation and infiltration. The movement of water within the soil after end of infiltration is called redistribution, since its effect is to redistribute soil water from upper layers of soil, wetted to near-saturation, to the lower layers. The rate of distribution depends on the soil properties, the groundwater depth, and the

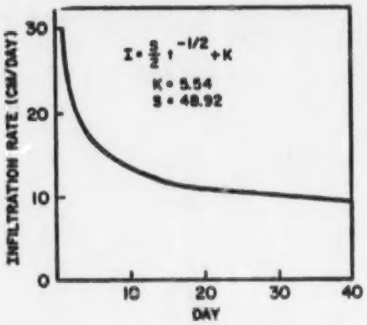

Figure 3. Infiltration Rate as a Function of Time

moisture content of the soil. The redistribution process also involves hysteresis, which complicates the redistribution process and makes it difficult to describe mathematically.

For this study, the redistribution process determines the time required for draining the excessive water in the soil. The faster the soil drains the excessive water, the earlier it can start the drying process. Normally, whether the infiltration basin is ready for next effluent application depends on the moisture content of the top soil. As a result, only the redistribution process of top soil is considered for this study. The depth of the top soil can be considered as root zone or tillage zone normally observed in the field. For this reason, we assumed that the redistribution in the top soil will become negligible when the soil water content reaches field capacity. Field capacity is defined as the amount of water that a well drained soil retains about 48 hours after being thoroughly wet. Thus, we considered that the redistribution process would take two days after infiltration ceases. We further selected 0.3 volumetric water content as the field capacity for this study, after which we assumed that the redistribution process ceases and drying process starts.

Evaporation and Drying

Evaporation

The loss of water through evaporation occurs during the period when effluent is ponded in the infiltration basin. U.S. Weather Bureau publications were used for the mean monthly rate of evaporation. In the simulation, evaporation ceased as soon as the ponding water was depleted. Water losses to the air were then considered to be from drying.

Drying

Drying occurs in two distinct stages. First, when there is ample water in the soil, the drying rate is constant and is determined by external and soil-surface conditions, rather than conductive properties of the soil profile. Constant-rate drying generally occurs while the soil water undergoes the redistribution process. After the soil reaches field capacity, the drying process enters into second stage, which proceeds at a rate lower than the constant rate and is controlled by the conductive properties of the soil profile. The second stage is called falling-rate drying. A study of evaporation from bare soil was reported by Gardner and Hillel[5], who stated that the drying rate can be expressed as:

$$E = D(\theta)\ W\pi^2 / 4L^2 \qquad (10)$$

where E is drying rate in cm/day, $D(\theta)$ is the diffusivity corresponding to the average water content of soil columns in cm^2/day, and W is the volumetric water content in cm for a soil column L cm long.

We confined ourselves to investigating the top 30-cm layer of soil because in practice, this is the layer that dictates whether the basin is dried to a degree ready for next application of effluent. As shown in Figure 4, we assumed that the drying process starts when the soil is at field capacity, after which the water loss through drying would follow Equation (10) until a 0.1 volumetric water content is reached for the top 30 cm of soil. We assumed that the constant drying rate is equal to drying rate determined by Equation (10) at volumetric water content = 0.3, or the evaporation rate, whichever is smaller

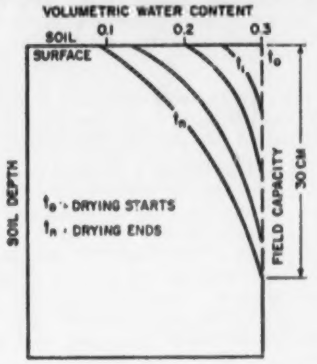

Figure 4. Illustration of Drying Process in the Soil

Diffusivity of the soil is generally measured experimentally. Testing procedures are available from many technical papers and soil and water textbooks. Figure 5 presents the diffusivity used in this study as a function of water content, while Figure 6 presents the drying rates determined by Equation (10) for soil water content ranges pertinent to the drying period.

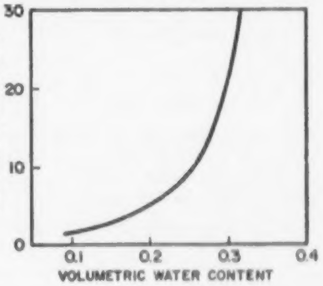

Figure 5. Diffusivity-Water Content Relationship

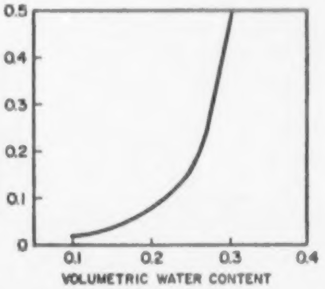

Figure 6. Drying Rate-Water Content Relationship

Simulation

Procedure

Once the mathematical equations for the various components of the land disposal process were formulated, simulation of secondary effluent disposal on an infiltration basin was initiated. Input data were local daily rainfall and evaporation, and parameters to describe the infiltration and drying properties of the soil, including sorptivity, conductivity, and diffusivity.

After obtaining the necessary input data and parameters, the simulation was conducted on a digital computer according to the following steps:

- The simulation started at the beginning of each day with the addition of the daily rainfall on the surface of the applied effluent. If it was not raining, a zero amount of rainfall was added. The depth of effluent on the next day was obtained by subtracting the amount of water lost by infiltration and evaporation during the previous day. This procedure was repeated until no more ponding effluent remained on the surfacee of the basin.
- After infiltration ceased, two days were added for redistributing excessive water in the top 30 cm of soil to the field capacity. In case rain occurred within the two days, the amount of the total rainfall was compared with the water lost through constant-rate drying and infiltration. If it was larger than that lost by drying and infiltration, the excessive rainwater was considered to be ponded on the surface, and the simulation returned to Step 1. If it was smaller, then an extra day was added to account for the additional infiltration process. The water lost through drying was determined utilizing the drying equation at a volumetric water content of 0.3.
- After reaching field capacity, loss of soil water through drying occurred. If rain occurred during this period, the amount of rainfall was compared with the existing water content of the soil to determine whether it would increase the soil moisture content, or return the soil water to Step 2, or even to Step 1. The entire process stopped when the volumetric water content of the top 30 cm of soil reached 0.1.

After completion of the above three steps, effluent was applied to the basin again and the above steps were repeated. This process was repeated until the simulation progressed to 20 years.

Five locations were chosen to represent different meteorological conditions: Phoenix, San Francisco, Miami, Boston, and Duluth. In recognition of the difficulty in applying effluent on land in freezing weather, the normal freezing period for Boston and Duluth was excluded from simulation. As a result, 8 months out of a year were used for disposal in Boston, and 6 months for Duluth.

The total effluent to be disposed of for each application was chosen as 200, 500 and 1,000 cm per unit area for all locations.

Output

The output of this simulation was a random variable, the time required for disposing the effluent on the basin, and its associated frequency of occurrences for the simulation period of 20 years. A sample output is shown in Table 2. It shows that if applying 500 cm of effluent on the basin in Miami, once in 20 years it would be possible to dispose of the effluent within 35 days, 6 times it would be possible within 42 days, and so on. The mean period between two successive applications is shown to be 64.2 days. The output for the simulation in other areas are summarized in Table 3.

Table 2. Simulation Output for Miami for Applied Depth = 500 cm.

Time reqd. day	No. of Occurrences	Time reqd. day	No. of Occurrences
35.0	1.0	59.0	80.0
42.0	6.0	60.0	20.0
43.0	2.0	71.0	1.0
46.0	1.0	80.0	1.0
52.0	1.0	81.0	1.0
57.0	2.0	82.0	3.0
58.0	4.0	83.0	2.0

Table 3. Mean Disposal Time for Effluent Applied on Infiltration Basin

Location	Mean Disposal Time (Days)				
	Application Depth (cm)				
	1000	500	200	100	50
Boston	103.3	56.9	27.0	18.2	16.6
Duluth	109.7	54.6	26.5	18.8	14.2
Miami	136.6	64.2	33.0	24.8	22.4
San Francisco	128.1	71.2	33.2	26.7	22.4
Phoenix	91.5	40.4	18.0	-	-

Applications

The major application for the output of this simulation was to determine the liquid loading rate, which in turn was used to size the required field area in which the disposal process actually takes place. For example, Table 3 shows that in the Miami area it takes an average of 64.2 days to dispose of 500 cm of effluent, therefore the liquid loading per year is:

$$\frac{365}{64.2} \times 500 = 2843 \text{ cm/yr} = 93 \text{ ft/yr} \qquad (11)$$

and the field area required based on the liquid loading is:

$$\text{Field area(acres)} = \frac{1118\ Q}{L}$$

where Q = flow rate of plant effluent, MGD; L = annual liquid loading, ft/yr. Therefore, for a 1-MGD plant, the required field area would be 12 acres. The actual system may be constructed as a series of infiltration basins. The effluent would be pumped into the first basin to a predetermined depth. The basin would be kept flooded until the total effluent reaches 500 cm. Then the basin would be left to dry out. The effluent would be applied to the basin again when the volumetric water content in the basin reaches 0.1. The design for this particular example seems quite adequate, because based on the 20-year simulation, the actual disposal time is larger than the average value of 64.2 days only nine times.

The liquid loading rates for other areas are presented in Tables 4 to 6, which also list the required field area for a 1-MGD plant.

Discussion of Results

The results indicate that the required field area for an infiltration type of land disposal system differs depending on the weather conditions and soil properties. For example, under the same conditions, an infiltration basin in the Miami area requires about 50% more area than one located in Phoenix.

The study also indicates that the required field area decreases if the basin is kept flooded longer. For example, the required field areas for a 1-MGD plant in the Miami area are 12.8, 12.0, and 15.4 acres

Table 4. Liquid Loading Rates and Required Field Areas for 1-MGD Plant at Various Locations

Effluent Depth per Application: 100 cm (32.8 ft)

Location	Liquid Loading Rate (ft/yr)	Field Area (Acre)	Storage* Area (AC-ft)
Boston	76.2	14.7	368
Duluth	53.8	20.7	552
Miami	87.7	12.8	Not required
San Francisco	93.5	12.0	Not required
Phoenix	130.9	8.5	Not required

*Storage area for effluent during the freezing period.

Table 5. Liquid Loading Rates and Required Field Areas for 1-MGD Plant at Various Locations

Effluent Depth per Application: 500 cm (16.4 ft)

Location	Liquid Loading Rate (ft/yr)	Field Area (Acre)	Storage* Area (AC-ft)
Boston	69.2	16.0	368
Duluth	54.1	20.7	552
Miami	93.3	12.0	Not required
San Francisco	84.1	13.3	Not required
Phoenix	149.3	7.5	Not required

*Storage area for effluent during the freezing period.

Table 6. Liquid Loading Rates and Required Field Areas for 1-MGD Plant at Various Locations

Effluent Depth per Application: 200 cm (6.6 ft)

Location	Liquid Loading Rate (ft/yr)	Field Area (Acre)	Storage* Area (AC-ft)
Boston	58.3	19.2	368
Duluth	44.6	25.1	552
Miami	72.6	15.4	Not required
San Francisco	72.1	15.5	Not required
Phoenix	133.1	8.4	Not required

*Storage area for effluent during the freezing period.

corresponding to effluent depth per application of 1000, 500, and 200 cm. In other words, the longer the basin is flooded, the more effluent is infiltrated into the ground, and consequently smaller field area is required. However, this does not mean that we should select the longest flooding time in order to have the highest liquid loading rate, because the liquid loading rate alone is not sufficient to design the system. The ability of soil to renovate the effluent and to avoid excess nitrogen loadings on the groundwater should be considered. The determination of water quality loading rates is beyond the scope of this paper.

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COMPUTER SIMULATION OF LONG-TERM SECONDARY IMPACTS OF WATER AND WASTEWATER PROJECTS

Gerald A. Guter, Ph.D.
Director of Environmental Studies
Boyle Engineering Corporation
Newport Beach, California

John F. Westermeier
Biologist
Boyle Engineering Corporation
Newport Beach, California

Thomas C. Ryan
Environmental Planner
Boyle Engineering Corporation
Newport Beach, California

Summary

Applications of the KSIM technique were made in the course of environmental studies for water and wastewater projects. The National Environmental Policy Act mandates a systematic interdisciplinary approach which will insure the integrated use of natural and social sciences and the environmental design arts in planning and in decisionmaking which will have an impact on man's environment. KSIM is being employed as a part of this interdisciplinary approach. This application of KSIM requires modification of published techniques for water resource planning and adaptation to the cases discussed.

The computer simulation, as applied to three water and wastewater projects, are discussed herein. These projects include an Areawide Facilities Plan for the Las Virgenes Municipal Water District in Los Angeles and Ventura Counties, California; a Master Plan of Water and Reclamation Facilities for Los Alisos Water District, Orange County, California; and an irrigation project on the Colorado River Indian Reservation in western Arizona. In considering the application of KSIM to the above projects, major advantages, acceptability to reviewers and agencies, types of projects to which KSIM appears applicable, and further research on the methods are discussed.

Background

Section 102 of the National Environmental Policy Act sets forth broad and sweeping policies for all agencies of the Federal government to:

(A) Utilize a systematic, interdisciplinary approach which will insure the integrated use of natural and social sciences and the environmental design arts in planning and decisionmaking which may have an impact on man's environment.

(B) Identify and develop methods and procedures, in consultation with the Council on Environmental Quality established by Title II of this Act, which will insure that presently unquantified environmental amenities and values may be given appropriate consideration in decisionmaking along with economic and technical considerations.

(C) Include in every recommendation or report on proposals for legislation and other major Federal actions significantly affecting the quality of the human environment, a detailed statement which is now commonly referred to as an Environmental Impact Statement.

Litigative activity over past years has centered around implementation of Section 102(C). Case law and guidelines prepared by the Council on Environmental Quality and by the Federal agencies have left little doubt about certain aspects of Environmental Impact Statement (EIS) preparation. They deal mainly in subject matter or required contents, format, and procedures of review, however; and give little guidance for implementing Sections 102(A) or (B).

Section 102(A) mandates the use of the interdisciplinary approach which insures integration of the disciplines. This implies the numerous expertise must be communicable to an integrator or one trained as a generalist, or the experts must learn to communicate among themselves. In either case, communication interdisciplinary in nature is necessary within the decisionmaking body. The use of several disciplines, however, is a difficult and time-consuming task.

Section 102(B) mandates an additional difficult task for the agencies preparing environmental documents. This section requires that "unquantifiable environmental amenities and values may be given appropriate consideration in decisionmaking." The Tenth Circuit's decision in Trout Unlimited vs. Morton (7 ERC 1321) touched upon the importance of the unquantifiable. This court said that in most projects, "the ultimate decision to proceed . . . is not strictly a mathematical determination. Public affairs defy the control that precise quantification of its issues would impose."

The preparation of environmental documents pursuant to NEPA and the so-called "little NEPA" legislation adopted by states requires the development of methodologies to effectively implement the above NEPA sections. The Environmental Studies Department of Boyle Engineering Corporation is pioneering the use of a computer simulation procedure for EIS preparation which was developed for integration of the disciplines. The methodology described in this paper allows for a structured and sophisticated consideration of the numerous complex relationships of a project or alternative and its environment, yet is so structured to allow the integration of both "hard" and "soft" data.

Description of Simulation Model

Because of their mathematical nature, most simulation models tend to be excessively numerical. Variables which are readily quantified exclude variables which are subjective or intuitive but which may be just as important. For example, wastewater collection network parameters, treatment plant capacity, and discharge requirements are included in the scope of planning a wastewater treatment system. However, subjective or semi-quantitative considerations such as local planning policy, environmental quality, and stimulus to land development can easily become the controlling factors in the choice of an alternative system.

The methodology of the simulation, taking into consideration both quantitative and qualitative variables and applied to cases described below, was developed by Kane, Vertinsky, and Thomson[1] and applied to water resource planning. For a detailed account of the mathematical treatment of the model, the reader is referred to the above basic reference, as well as reports by Krusic[2] and Suta[3]. One of the advantages of the Kane Simulation Model (KSIM) is that a detailed mathematical knowledge of the model is not required to use the model. Thus, a barrier is removed between the disciplines who jointly participate in the construction of the model variables and the simulation modeling by use of a simplified simulation language.

KSIM mathematics has the following properties:

(1) System variables are bounded. It is assumed that any variable of human significance cannot increase indefinitely; there must be distinct limits. In an appropriate set of units these can always be set to one and zero.

(2) A variable increases or decreases according to whether the net impact of the other variables is positive or negative.

(3) A variable's response to a given impact decreases to zero as that variable approaches its upper or lower bound. It is generally found that bounded growth and decay processes exhibit this sigmoidal character.

(4) All other things being equal, a variable will produce greater impact on the system as it grows larger.

(5) Complex interactions are described by a looped network of binary interactions.

Representative previous applications of KSIM include Impact of Canadian Water Sales to the United States (Kane), Implications of a U.S. Deep Water Port Policy (U.S. Army Corps of Engineers), Sensitivity of Alternative Manpower Policies (U.S. Office of Naval Research), and Effects of a "Make or Buy" Research Policy (Policy and Planning Directorate, Canada).

We use the following procedure to apply KSIM as a part of the environmental impact reports or statements. The most appropriate portions of a study are those in which long-term relationships between the proposed project, its alternatives, and unquantifiable values must be analyzed. The steps are as follows:

Step 1: Assignment and Preparation of Team Members. Normally all specialists who participate in the preparation of the draft statement are assigned to the KSIM team. These are staff scientists, engineers, and planners of varying backgrounds and expertise involved in the major subject areas of the EIS. The individuals work together in various studies in support of the EIS and meet frequently to discuss the results of their studies. Thus, each is familiarizing himself with the proposed project, the environment of the project, and the alternatives under consideration. He is also learning to communicate with his team members. These researchers represent a core group. Other experts also familiar with the project area may join the core group at a later date. These may be lead agency staff members or the decisionmakers themselves.

Step 2: Identification of Variables. Critical long-term variables are identified and defined as precisely as possible. One variable must represent the proposed project or alternative. The definition of the variable is separated into its quantitative and qualitative components.

Step 3. Set Initial Values. A well defined variable will lend itself to setting an initial value. An estimate is made of the maximum growth level the variable could achieve. For example, if the variable is population, the initial value is the present fraction of the ultimate population.

Step 4. Cross-Impact Analysis. KSIM requires that two matrices be completed for the simulation. One of the matrices represents the long-term (Alpha) relationship between variables and the other represents the short-term (Beta) relationship. The matrices are constructed with each variable listed as a row and a column heading of a table. A basic assumption is that when one variable changes, it may increase or decrease each of the other valuables or it may have no relationship at all. Thus, "O," "+," "-" is assigned to each square of the matrices. Numerical values are assigned as a refinement.

Step 5. Computer Projection of Variables. Variables, initial values, and cross-impact values are typed into a computer with the KSIM program. The computer performs the interactive calculations and displays the projected changes in each variable over time. Team members may now modify and refine their model by changing variable definitions, initial values, and numerical cross-impact values or by choosing an alternative project. This refinement is repeated until the team members are satisfied that their projections and inputs are reasonable.

Step 6. Interpretation of the Projection. Major trends which appear in the projections and some analyses of the key factors, and issues which bring about those trends, can now be discussed using the projections as a basis for the discussion. Differences in the long-term impacts between the various alternatives can also be analyzed and discussed.

Examples of Applications of KSIM To Environmental Studies

The application of the KSIM procedure to preparation of environmental studies has been demonstrated in three water and wastewater management related projects in the past year. A fourth study application is currently under way. Described briefly below is the manner in which KSIM methodologies were applied to the various studies.

An EIS was initiated to evaluate an Areawide Facilities Plan of wastewater collection, treatment, and disposal facilities for the Las Virgenes Municipal Water District. The 118,000-acre service area of the District included coastal Malibu, portions of the Santa Monica Mountains, and inland areas of western Los Angeles and eastern Ventura Counties, California. The issues of population growth and land use presented unusual problems due to conflicting philosophies within the region. Population growth had been rapid and was considered desirable in the inland urban areas, whereas the coastal portions of the study area had defeated sewer bond issues (presumably on alleged growth-inducing impact) three times since 1966. KSIM was employed to model the long-term effects of implementing the Areawide Facilities Plan.

The KSIM team consisted of the staff of the Department of Environmental Studies. Staff members included specialists trained and experienced in the fields of water quality and reclamation, public health, social services, local and regional planning, ecology, and environmental geology.

Nine variables were defined and initial values set by the team according to procedures outlined in the previous section. They are given below:

Population (POP) represents the number of people living in the study area. An initial value of 15 percent was established.

Pollution (POL) indicates the level of air, water and noise pollution in the study area. The initial value of 45 percent represents the ratio of the present measured levels of the three pollutants to the regulatory standards set for maximum limits.

Desirability (DES) denotes the general attractiveness of the study area based on such factors as aesthetics, amenity, and quality of life. Largely a qualitative determination, the study area was given an initial value of 70 percent.

Urban Services (US) measures the quality and quality of public services such as schools, police, fire protection, and utilities provided to area inhabitants. Services were judged more than adequate as indicated by an initial value of 20 percent (5 percent above population).

Resource Consumption (RC) represents the total amount of energy and water consumed in the study area. The initial value of 11 percent is the ratio of present usage to that required by the ultimate population anticipating the effect of current and future energy conservation measures.

Residential Density (RD) indicates the ratio of high density urbanization to developed land, initially estimated at 25 percent.

Employment Dispersal (ED) is the relationship of distance between places of employment and residence. The initial value of 27 percent is the quantitative estimate of the ratio between maximum and existing distance driven to work.

Wastewater System Capacity (WSC) represents the proposed project. The initial value of 9 percent is the existing fraction of ultimate projected wastewater treatment capacity.

Cost of Living (COL) is probably the most qualitative of all variables. The initial value of 20 percent was based on the assumption that the cost of living would not exceed five times its present value.

Through cross-impact analysis, the Alpha and Beta matrices were completed and checked for obvious errors. The derived values were tested on the computer and subsequent refinements were made. Tables 1 and 2 show the Alpha and Beta matrices which produced the regional model depicted in Figure 1.

Table 1. Alpha Matrix of Long-Term Impacts

	POP	DES	POL	US	RC	RES	ED	WSC	COL
POP	+2	+1	- .5	+1	0	- .1	-1	+ .25	-1
DES	-1	+ .5	-1.5	+1.3	0	-1	-1	+1.7	- .5
POL	+2	0	+ .5	+ .5	+2.2	-1	+1.2	- .7	- .5
US	-1	+1	0	0	0	-1	0	0	+ .8
RC	+1.5	0	0	+1	+ .5	- .5	+1.5	+1	-1
RES	+2	-1	+ .5	-1	- .3	+ .5	0	0	+1
ED	0	- .5	0	0	0	- .2	0	0	- .5
WSC	+1.5	+ .2	0	+ .5	+1	- .5	0	0	- .5
COL	0	+ .8	0	+ .9	+ .6	-1	+ .5	+ .6	0

Table 2. Beta Matrix of Short-Term Impacts

	POP	DES	POL	US	RC	RES	ED	WSC	COL
POP	0	0	- .2	0	0	0	- .3	0	0
DES	+ .5	+ .1	-1.5	+ .3	0	- .8	0	+ .1	- .2
POL	+2	0	+1	0	+1.6	- .4	+1	-1.5	0
US	-1	0	+1	0	- .5	0	0	0	0
RC	+1.5	0	0	0	-1	0	+1	0	-1.3
RES	-1	+ .1	0	0	0	+ .3	0	0	0
ED	0	0	0	0	0	0	0	0	- .1
WSC	-1	0	0	0	- .5	+ .5	0	0	0
COL	+ .5	0	0	+ .5	+ .7	0	0	0	0

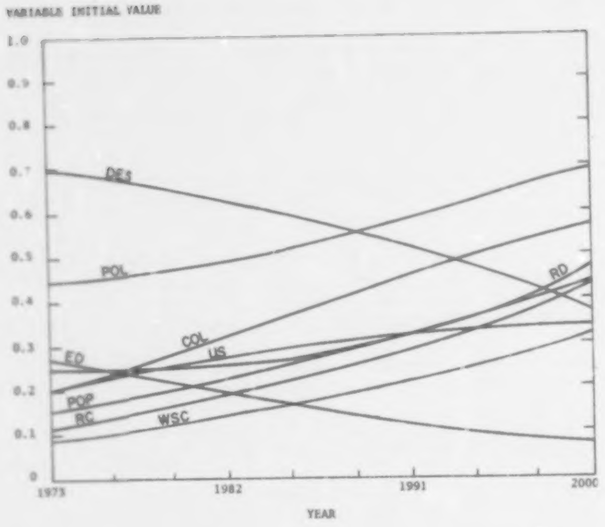

Figure 1. Regional Model, Areawide Facilities Plan

The simulation indicates continued urbanization in the study area, shown by the increases in population, urban services, and residential density. The fact that urban services increase slightly is an indication that the area may be able to retain much of its rural character.

Resource consumption increases at a rate slightly greater than the population, indicating a slight increase in per capita consumption. The continued rise in pollution can be directly tied to its strong relationship with both population and resource consumption. The steady decrease in employment dispersal indicates an increase in the number of employment centers in the project area. (The area has virtually none at present.) Joining employment dispersal in an overall decline over the planning period is desirability. The decline is attributable mainly to increases in population and pollution. Cost of living does interact here, also tending to reduce desirability. The increases in population, resource consumption, and urban services indicate future growth, which are accommodated by increased wastewater system capacity. The demand for wastewater treatment facilities for the year 1987 in the simulation does not rise above the capacity that would be provided by the proposed project.

KSIM was again employed in association with an environmental impact report for the Master Plan of Water and Reclamation Facilities of the Los Alisos Water District, a 5,400-acre district located within a rapidly growing area of Orange County, California. Several constraints on growth exist within the district, including land use restrictions associated with the flight path of a military air base and lack of regional wastewater treatment and disposal facilities.

Team members participating in the KSIM analysis included members of the Department of Environmental Studies. District staff and the Board of Directors reviewed initial KSIM models and offered suggestions for refinement of the models. Nine variables defined for this study include the following:

Population (POP) is a quantitative variable of the number of people residing within the district.

Nonrenewable Resources (NRR) represents consumption levels of nonrenewable resources within the district including energy consumption and use of construction materials.

Public Services (PUB) reflects levels of public services including schools, parks, solid waste collection, police protection, public transportation, and social services.

Pollution (POL) variable is a semi-quantitative variable reflecting levels of water and air quality within the district.

Natural Resources (NAT) reflects both qualitative and quantitative, ecological, agricultural, mineral, and archaeological resources of the district.

Economic Resources (ECO) reflects both quantitative and qualitative aspects of economic activity within the district including property values, business activity, family income, and employment.

Desirability (DES) is a qualitative variable reflecting the characteristic which may cause people to desire living in an area. Examples of these characters include levels of public services; closeness to work, shopping, and friends; quality of schools; and aesthetic qualities.

Reclamation (REC) is a quantitative variable representing the amount of wastewater generated within the district that must be reclaimed.

Water Consumption (WAT) is a quantitative variable representing the amount of water used within the district.

Three KSIM models were generated to reflect possible changes in land use and in wastewater treatment and disposal. The first model (Case 1) was the more conservative case reflecting current land use restraints and wastewater treatment and reclamation near or within district boundaries. Case 2 reflected the addition of some capacity in regional treatment and disposal facilities. Case 3 reflected a situation where land use restraints associated with the flight path of the military air base were liberalized and regional wastewater treatment was available.

Alpha and Beta matrix values for Case 1 are in Tables 3 and 4. Alpha and Beta values for Cases 2 and 3 were similar; however, the initial value for reclamation was lowered to reflect capacity in regional wastewater treatment and disposal in Cases 2 and 3. The initial value for population was also lowered in Case 3 to reflect a potential higher ultimate population.

Table 3. Alpha Matrix for Case 1

	POP	NRR	PUB	POL	NAT	ECO	DES	REC	WAT
POP	+2	- .2	+1	+ .2	+ .3	+2.5	+2	-1	+ .1
NRR	+2.5	+ .5	+ .5	+1	- .5	+1.5	+1	+1.5	+ .4
PUB	+ .5	+ .5	+ .2	+1	- .2	+1	+1.5	+1	+ .3
POL	+2	+1	- .3	+ .3	- .3	+ .5	+ .2	+ .3	+ .1
NAT	- .4	- .4	- .3	- .4	+ .5	- .5	+ .1	- .5	- .1
ECO	+2	- .3	- .2	- .4	- .2	+ .8	+1.5	- .8	+ .5
DES	- .2	- .1	+1	- .5	+ .5	+1	+1	- .4	+ .3
REC	+3.5	+1	+2	+1.5	- .3	+2	+1	+ .5	+2.5
WAT	+2.5	+1	+1.5	- .3	- .1	+1.5	+ .7	-1	+ .5

Table 4. Beta Matrix for Case 1

	POP	NRR	PUB	POL	NAT	ECO	DES	REC	WAT
POP	+2	- .5	+2	- .5	+ .3	+2.5	+2	+2	+ .1
NRR	+ .8	+ .5	+ .5	+1	-1	+1.5	+1	+1.5	+ .3
PUB	+1.5	+ .5	+ .5	+1	- .2	+1	+ .8	+ .5	+ .5
POL	+ .5	+1.5	- .2	+ .1	- .1	+1	+ .1	+ .5	+ .1
NAT	-2	- .5	- .1	- .4	+ .5	-1.5	+ .2	-1	- .1
ECO	+2	- .5	- .2	- .5	- .5	+ .5	+1	-1	+ .5
DES	- .5	- .4	+1	- .5	+ .5	+1.5	+ .8	- .5	+ .3
REC	+ .3	+1	+1	+1.5	- .3	+1.5	+1.5	+ .5	+2.5
WAT	+2.5	+1	+1	- .3	- .3	+1	+ .7	- .8	+ .5

Computer projections of each variable for Case 1 are shown in Figure 2. Population rises to the approximate levels predicted by current land use elements. Nonrenewable resource consumption increases in the district, reflecting increased urbanization. Public service levels rise slightly. Pollution levels increase over time reflecting air quality degradation in the region. As urbanization increases, natural resources decrease in the district. Economic resources rise steadily over time. Desirability remains at approximately the same level. Reclamation and water consumption increase in relation to population increase. Computer projections of variables for the other two cases were similar to Case 1 with higher population, reclamation, and water consumption, and a sharper decline in natural resources.

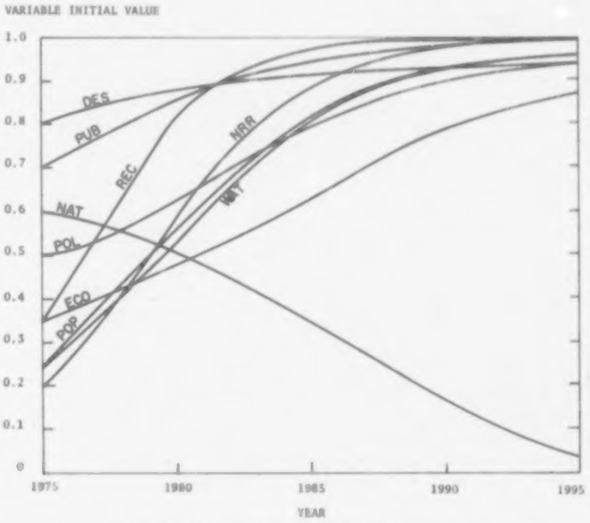

Figure 2. Regional Model for Case 1

A brief description of KSIM and the results of the computer simulations were included in the environmental impact report for the district's Master Plan. Public agencies, organizations and individuals reviewing the EIR had no adverse comments to offer in regard to the use of KSIM.

Use of KSIM by the Department of Environmental Studies has not been limited to wastewater projects. KSIM has provided valuable assistance in analyzing environmental impacts associated with expanded agricultural development on the Colorado River Indian Reservation in western Arizona. Team members were limited to the staff of the Department of Environmental Studies. Variables selected for the analysis included: Indian Self-determination (ISD), Agriculture (AG), Resource

Consumption (RC), Scientific Relationships (SR), Pollution (POL), CRIT System Procedures (CSP), Quality of Social Services (QSS), Employment (EMP), and Tribal Income (TI).

Computer projection of these variables is shown in Figure 3. Several trends are apparent in this simulation. Indian self-determination rises possibly in response to higher tribal income brought about through increased agriculture and employment. Resource consumption also increases in response to increased agricultural development. Increased agriculture also appears to result in increased pollution levels and lowering of scientific relationship values. Quality of social services is projected higher although government role (CRIT System Procedures) in the reservation is decreased.

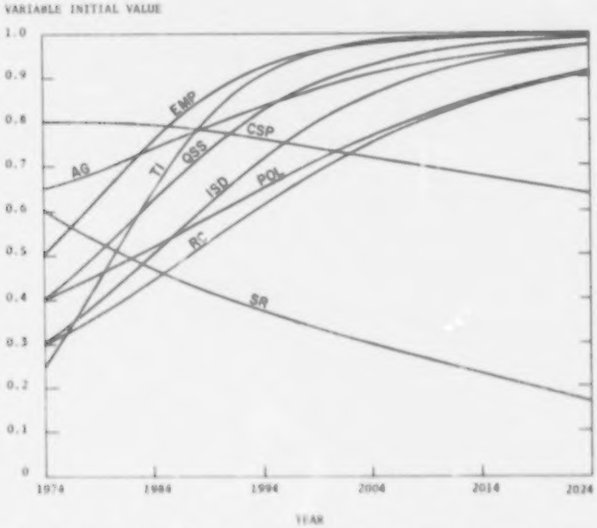

Figure 3. Model for Colorado River Indian Reservation

The Department of Environmental Studies is currently applying KSIM to the evaluation of environmental aspects of a water-oriented recreational development. Variables including recreation, resource consumption, environmental quality and jurisdictional framework have been defined for this simulation.

Operational Aspects and Implications of Use

The application of KSIM to appropriate projects has distinct functional advantages. It allows a multidisciplinary interchange as mandated by current environmental legislation, and provides a sound basis to decisionmaking through the interactions of the panel approach. Its use of cross-impact analysis encourages disciplined inquiry and allows decisionmakers to appreciate the magnitude and complexity of factors affecting planning decisions. As it provides a model of the future, it may be periodically checked to determine if adopted policies are having the effects initially perceived. Future changes in goals and policies can be readily integrated into the KSIM model through ongoing refinement.

Additionally, KSIM has advantages related to EIR/EIS processes. Evaluation of long-term, secondary, environmental impacts as required by NEPA and other acts is greatly facilitated by the KSIM projection. Displaying the projections at work sessions or public hearings and soliciting comment on the models can provide decisionmakers with a unique way of involving the public in the planning process.

KSIM is attractive to many reviewers and public agencies as participation in cross-impact analysis does not require a highly technical background. Because of this relative simplicity in use, decisionmakers and other interested parties can actively participate in the formation of the simulations. However, use of KSIM for many agencies is limited due to the availability of necessary data processing equipment. Active participation by many decisionmakers is also hampered by the time required for completion of both Alpha and Beta matrices by the KSIM panel.

We believe KSIM has wide applicability for environmental studies on many types of projects in addition to those discussed in this paper. Generally, KSIM can be applied to projects where impacts of a project go well beyond the immediate time frame. It is particularly well suited for projects requiring master planning techniques,as KSIM itself is a planning exercise. We believe KSIM will be more commonly used for projects which require a decision about implications of future growth.

We are currently researching methods to modify, monitor, and refine the KSIM procedure so that it can be more easily implemented. One approach is to reduce the time required to formulate and run a simulation. Ways in which this may be accomplished include: the composing of checklists of typical variables for specific types of projects, standardizing and refining methods for setting variable limits and determining initial values, and adjusting the program and procedure to require only the Alpha cross-impact matrix.

It may be possible to save much panel discussion time by bringing the decisionmakers into the exercise at a later stage of the simulation. Decisionmakers would then have more of an evaluative function since a core group would have already defined variables and set initial values. The use of questionnaires is also being investigated as a way to document the input of KSIM team members who cannot participate in the discussion in person.

Future research of the KSIM procedure is needed to substantiate the accuracy and validity of the model. This can only be done through long-term monitoring and evaluating of a KSIM model, and subsequent revision of the procedure. As with any planning tool, however, KSIM's real benefit is not in predicting the future but in facilitating the formulating of policy which will at least set a rational course of action towards the future.

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A CRITICAL APPRAISAL OF MATHEMATICAL MODELS FOR LAND SUBSIDENCE SIMULATION

E. John Finnemore and Robert W. Atherton
Systems Control, Inc.
Palo Alto, California

Summary

Land subsidence can have a major environmental impact resulting from the withdrawal of geofluids: oil, gas, groundwater, or geothermal water and steam. While mathematical models for simulating land subsidence caused by pore fluid withdrawal are still in a relatively early stage of development and are not yet very numerous, the subject is drawing increasing attention. Documentation is available on two simple and nine advanced models of this type, and additional models under various stages of development were identified. The appraisal of such models reported here required an examination of the physics included, the model equations, the numerical methods, and the practical applicability of each. The status of this field and the need for further work are reviewed.

Background

Examples of major subsidence resulting from the withdrawal of petroleum, groundwater, and geothermal fluids are respectively: 8.8m vertical and 3.6m horizontal movement over the Wilmington oil field, Long Beach, California; 8.8m vertical movement in the San Joaquin Valley, California; and 4.5m vertical and 0.8m horizontal movement at the Wairakei geothermal field in New Zealand. Numerous instances of lesser subsidence have occurred around the world.[1]

The total environmental impact of subsidence obviously depends upon the geographic and economic development of the site. In populated areas, roads, railroad tracks, sewers and drains, power lines, pipelines, wells, airfields, houses, and buildings may be damaged. In rural areas, dams and levees, irrigation channels, agricultural drains, wells, electric transmission towers, vegetation patterns, and crop irrigation patterns may be affected. Along coastlines and rivers the areas subject to flooding may be altered and increased, and drainage paths may be changed. In any location, the incidence of minor earthquakes may be affected. Within the producing field itself, wells and well casings, pipelines, and plant (if any) may be damaged, and the storage and transmissivity of the producing porous medium (fluid reservoir) may be reduced. It must be noted that the resulting bowl-shaped surface depressions which usually form may be significantly offset from the producing wellfield, as occurred at Wairakei. Also, for a number of the impacts just mentioned, horizontal ground motion (not predictable by one-dimensional subsidence models) can have far more serious effects than vertical motion.

Models are employed for two reasons: they provide a mechanism with which to improve our understanding of the nature and behavior of a producing field, and they provide a means for predicting subsidence and for investigating alternative schemes for subsidence mitigation. As early as 1925, while providing an understanding of the consolidation of soils for the first time, Terzaghi deemed theories of models to be among the most important and indispensible engineering tools.[2]

The work reported here was performed as part of a study of subsidence associated with geothermal development, supported by the National Science Foundation. The models reviewed in that study also included certain other non-subsidence models, which have frequently been incorporated into the subsidence models. The work was accomplished by a review and analysis of the published and unpublished literature on models for subsidence caused by any type of geofluid withdrawal. This was supplemented by discussions and interviews with researchers in the field of subsidence modeling, and by attendance at numerous seminars and symposia where these topics were considered.

Model Appraisal

Formulating a mathematical model for land subsidence is no small undertaking. As usual in modeling geophysical processes, the accuracy of the model is limited by the ability to describe the detailed structures provided by nature. Even when the scope of the modeling effort is reduced, two major problems remain: the question of data availability and the problem of computational tractability. It is not clear whether the data base for a large-scale model is available at this time. With regard to computational tractibility, a comprehensive three-dimensional reservoir subsidence model would tax even today's large computers.

Despite the drawbacks listed above, models are invaluable as a means of studying a phenomenon, correlating data, identifying the most crucial data needs, or extrapolating to unknown conditions. In studying subsidence, we have been compelled to rely on a hierarchy of models rather than a single definitive model. Our appraisal has consisted of three parts: (1) a study of the simplest class of subsidence models, (2) an investigation of the form of an advanced subsidence model which would provide the minimum predictive capability, and (3) a study of the state-of-the-art in subsidence modeling.

Simplified Subsidence Models

Simplified models serve two purposes. First, they provide models which can be used independently of large computers and program decks. Thus, they provide an inexpensive means of making a first estimate of subsidence, and they provide a vehicle for the non-expert in solid mechanics to obtain an understanding of the subsidence process. Second, the site data required to use a simple model are limited and more likely to be available.

Simplified subsidence models have been developed by adapting the work of Geertsma.[3] These simplified models will be a key portion of a subsidence handbook being developed to provide a guide to the analysis of potential subsidence associated with geothermal development.[4]

The simplest compaction model can be expressed as follows:

$$\Delta H = H\, C_m\, \Delta p$$

This simple equation illustrates the fundamentals of compaction. The compaction ΔH is the product of the reservoir thickness H, the reduction in pore pressure Δp, and the compaction coefficient C_m. Therefore, as Geertsma pointed out, compaction can occur in well consolidated reservoirs, if they are thick and experience a large decrease in pore pressure.[3] Slightly more sophisticated models have also been presented in which C_m is calculated using an integral over total effective stress.

This compaction equation alone does not account for response of the overburden to reservoir compaction; it is the surface deformation that is evident as subsidence. A simple overburden model is also available.[3]

Description of an Advanced Subsidence Model

In modeling subsidence, we are interested in describing the sinking of the earth's surface due to adjustments in the subterranean material stimulated by the withdrawal of geothermal fluids. Since the fluid withdrawal is the subsidence stimulus, the first requirement is for a well-bore model and a reservoir model to relate the pore-pressure distribution in the reservoir to the rate of withdrawal at the surface. Since reservoir compaction is the precursor of subsidence, a second need is a constitutive equation, a model for mechanical behavior, for the reservoir material. These two models must be coupled (interactive), as compaction affects the porosity and permeability of the reservoir.

Two additional distinct material models will be required: one for clays and one for the overburden. Clays in communication with the reservoir will also undergo reduction in pore pressure, and consequently will compact, though usually with considerable time delay. The overburden, experiencing a change in stress at the reservoir boundary, will deform; the deformation of the overburden can be treated as an elastic material. The all-important reservoir will likely require treatment as a plastic material in order to account for the well known irreversible nature of compaction.[5] The same argument holds for clays. The exact form of the required two plastic constitutive relations is yet to be determined.

To summarize, an advanced subsidence model must include computer subroutines to generate the characteristic physical properties of the site. It should contain a well-bore model, a reservoir model, and three models of material behavior, i.e., for the reservoir, communicating clays, and the overburden. All models should be implemented using the best available numerical methods.

Survey of Subsidence Models

The recent interest in environmental aspects of land subsidence, and the increased availability of large computers, have provided incentives to the development of models for subsidence. A considerable number of these models are presently under continuing development. In addition, more subsidence models will be introduced by the plans to incorporate deformation models into many of the reservoir models (fluid flow, or fluid heat flow only) presently under development also; these future possibilities are not discussed here.

The survey reported here identified two simple and fourteen advanced models designed to simulate subsidence caused by geofluid withdrawal. The developers of these models and the applications for which they were designed are listed in Table 1. In the miscellaneous category, the first model has a general capability for any type of man-induced subsidence, and the second simulates natural geological subsidence in a basin experiencing sedimentary deposition. While much has been learned about the effects of groundwater withdrawal since Terzaghi described his consolidation theory in 1925, advanced models for simulating resulting ground deformation are seen to have appeared only after 1972. Mathematical models for computing land subsidence caused by the extraction of oil and/or gas from the ground were probably first formulated in the 1950's. The early models were all analytical models; a number of the more recent numerical subsidence models have been developed by petroleum company personnel, so that they remain proprietary. The recent upsurge of interest in alternate energy sources has stimulated the development of models for geothermal resources. However, only two geothermal subsidence models are, as of February 1976 near first-version completion, and neither of them has been tested in applications yet.

Table 1

MATHEMATICAL MODELS OF LAND SUBSIDENCE
CAUSED BY PORE FLUID WITHDRAWAL

TYPE	DEVELOPER(S)
Miscellaneous	Sandhu and Wilson (1970) Jacquin and Poulet (1970)
Groundwater	Gambolati, et al. (1973, 1974) Helm (1974) Narasimhan (1975)
Oil and Gas	*McCann and Wilts (1951) *Geertsma (1966) Geertsma and van Opstal (1973) Frazier (1973), Archambeau (1974) Finol and Farouq Ali (1975) Paris and Farouq Ali (ongoing) Kosloff and Scott (ongoing) Oil Companies (proprietary)
Geothermal	Pritchett, Garg, Brownell (1975) Lippmann and Narasimhan (ongoing) Safai and Pinder (ongoing)

*Simple models (remainder are advanced models)

Each of the models listed in Table 1 is discussed in the following paragraphs, in the same order.

Sandhu and Wilson developed a finite element method for the general analysis of land subsidence.[6] It permits the consideration in two or three dimensions of complex geometry, arbitrary time-varying boundary conditions, non-homogeniety as well as anisotropy, and non-linear and time-dependent material behavior including viscoelasticity, creep, temperature effects, residual stresses and plastic behavior.

Jacquin and Poulet developed a two-dimensional (axi-symmetric) computer model to study the hydrodynamic patterns in a naturally subsiding sedimentary basin.[7] With time and deposition of successive sand and clay strata, the depth of the conical-shaped basin increased and water was expelled from the clay. Fluid flow was horizontal in the sands and vertical in the clays.

Gambolati et al. developed a two-step mathematical model to analyze subsidence in the complex, unconsolidated aquifer-aquitard system underlying Venice, Italy.[8,9] The hydraulic pressures were calculated in a two-dimensional vertical cross section in radial coordinates in the first step by a model based on the diffusion equation, which was solved with a finite element technique. The values of the hydraulic heads in the aquifers were then used in the second step as time-dependent boundary conditions in a set of one-dimensional vertical consolidation models, which were solved with a finite difference technique. The compaction models are based on the one-dimensional form of the classic diffusion equation, written in terms of one unknown, the fluid potential, and employing only one elastic constant, the vertical compressibility, α. While the compressibility, α, of any layer may be a non-linear and irreversible function of the pressure head, at Venice the non-linearity was considered negligible. The irreversibility was provided by using two α values for each layer, one for compaction (preconsolidation) and another (about one-tenth as large) for expansion.

Although model calibration was hampered by the sparseness of the available data, the study was able to predict the results of alternative mitigation measures.[9] The main disadvantage of this model lay in the limitations imposed by the requirement of radial symetry. When using the two-α-value method described above, it is very important that the computer code should keep track of the past maximum effective stress at every point, and use the smaller (expansion) value for compression when the effective stress does not exceed the past maximum (preconsolidation) stress.

Helm has developed two one-dimensional mathematical subsidence models for groundwater withdrawal.[10-12] Cumulative compaction and expansion in a series of aquifers and aquitards was computed from the known applied stress history and from two storage coefficients (compressibility values), one for recoverable and the other for non-recoverable compression. By distinguishing between present effective stress and past maximum effective stress at any depth, these models employed the two storage coefficients in a manner very similar to that used in the model of Gambolati et al.[8,9] Non-recoverable compaction occurred only when the past maximum effective stress at any point was exceeded.

Helm's two models are also both based on the one-dimensional diffusion equation. One model assumes linear (not stress-dependent) coefficients, and the other assumes non-linear (stress-dependent) coefficients. Two transformations of applied stress enabled the non-linear formulation to be represented by an equivalent linear homogeneous formulation. Both models were solved by finite difference techniques.

The models were applied to a series of 21 aquitards at Pixley, in the San Joaquin Valley, California. There, continuous records of hydraulic head and compaction revealed 3.19 feet of compaction between 1959 and 1971, although there was no long-term decline of the groundwater level which experienced seasonal fluctuations of about 100 feet. The maximum error in the predictions of the non-linear model was 2.9% compared with 7% for the linear model.

Narasimhan has developed a subsidence model named TRUST.[13] TRUST will simulate transient groundwater motion in variably saturated, deformable, heterogeneous, isotropic, multidimensional, porous media. It incorporates a one-dimensional subsidence model employing Terzaghi's consolidation theory into a general three-dimensional, isothermal groundwater flow model. The non-linear governing equation employs the pore-pressure head as the dependent variable; it is solved using an integrated finite difference method.

TRUST was tested and verified on nine different problems. Applications involving deformation included:

- One-dimensional, time-varying consolidation of clay under a foundation load
- One-dimensional shrinkage of an active (bentonite) clay slurry, in which large volume changes can occur in very short times
- One-dimensional drainage (partially saturated flow) of a deformable sand
- Two-dimensional draining (both fully and partially saturated) flow in a deformable sand
- Two-dimensional drainage and deformation around a fresh excavation in soft clay.

McCann and Wilts developed two analytical models as part of a mathematical study of the oil-field subsidence in the Long Beach area.[14] At the time (c. 1950), it was decided that the only physical model which could logically describe the general known properties of the soil and be amenable to mathematical solution was one of a three-dimensional, homogeneous, isotropic elastic medium of semi-infinite (downward) extent. Solutions were obtained for motions (vertical and horizontal, as functions of depth) and stresses developed in such a medium under the action of general distribution of the two alternative types of idealized subsurface disturbance forces. These forces were intended to represent the effect of drops in the reservoir oil pressures, and ways were devised to obtain the forces from the pressure drops.

The first type of disturbance force was called a "tension center" (or "tension sphere"), and the second type consisted of a pair of equal vertical forces acting in opposite directions a short distance apart, consequently named a "vertical pincer."

Analysis yielded the stresses and deformations caused by such a single disturbance force. Employing the principle of superposition, arrays of tension centers and vertical pincers were sought which would yield the deformation observed at that time. The assumption of an elastic material is essential for the use of superposition, and McCann and Wilts themselves stated that the most serious difficulty with their analysis was the failure of the earth to behave like an elastic material. They found that the tension center model could be arrayed to fit all the observed deformation data to the accuracy with which they could be measured, while the vertical pincer model could fit none, and so they concluded that only the tension center model should be considered further.

Geertsma developed a three-dimensional analytical subsidence model for poro-elastic displacements around a contracting oil reservoir in a semi-infinite, homogeneous, isotropic rock medium.[15] It employed a "nucleus of strain" concept, and it integrated the resulting displacement function over the volume of a horizontal, disc-shaped producing reservoir. The same linear elastic properties were specified within and outside the reservoir, into which no natural recharge was allowed as the contained pore pressure was reduced, causing changes to both internal and external stresses and strains. Results of evaluations with this model indicated that notable subsidence (as opposed to compaction) can be expected only above large reservoirs consisting of highly compressible sediments and experiencing substantial pore-pressure reductions.

Geertsma's model (poro-elastic theory) described here, and McCann and Wilts' model (elastic theory) described previously, were reviewed, compared, related, and improved by Gambolati.[16] In particular, Gambolati demonstrated that Geertsma's model can be easily extended to incorporate heterogeneity of the reservoir (reservoir material more easily deformed than its overburden).

Geertsma and van Opstal evaluated conceivable numerical methods for calculating subsidence above oil or gas reservoirs of arbitrary three-dimensional shape and change in pressure distribution.[17] They concluded, in 1973, that the simplest method, which still provided a good overall impression of the spatial subsidence distribution, was one based on the linear elastic theory of nucleus of strain in the halfspace. Then tested a suitable three-dimensional finite element program named ASKA for such purposes, and obtained results which agreed quite satisfactorily with their analysis. They also developed another computer program to help integrate their nucleus-of-strain theory over a compacting reservoir of arbitrary shape, by dividing it up into a finite number of small parts. This latter approach they used to predict subsidence and horizontal displacement patterns over the Groningen gas field from 1975 to 2100.

Frazier and Archambeau developed an elastic reservoir model with interactive fluid flow and rock strain equations, which they applied to the Long Beach oil field with both production and injection.[18,19] It is an axi-symmetric or planar (two-dimensional) finite element model, which reduces to an implicit time-step scheme.

Finol and Farouq Ali developed a two-phase, two-dimensional black oil model for simulating reservoir production behavior and simultaneous ground deformation.[20] Reservoir compaction was described on the basis of reported experimental data, from which the surface subsidence was calculated using Geertsma's theory of poro-elasticity and nucleus-of-strain concept.[15] Fair results are obtained with a simulation of the production and subsidence history of an oil field on the Bolivar Coast of Western Venezuela.

Paris and Farouq Ali are presently extending the work of Finol and Farouq Ali described above, but no results have been published as yet.

Kosloff and Scott are developing a deformation model for the Wilmington oil field, which requires pore pressure histories as input data. This procedure has the advantage of removing uncertainties in the fluid-flow patterns caused by large variations in permeability, but it makes the model more difficult to use with future production schemes. They consider that soils exhibit plastic behavior from the start, and with stress they strain harden and eventually become elastic. Accordingly, they have used the plastic cap model as the basis of their constitutive relations. A two-dimensional, axi-symmetric version of this deformation model appears to have given good results for subsidence at Wilmington, in spite of the block-shaped zones in the reservoir formed by faults. They are now attempting to check these results with a three-dimensional version of the model.

Oil Companies are known to have various models for simulating subsidence over oil and gas fields and in permafrost. Because of their proprietary nature, few details are available.

Pritchett, Garg, Brownell and others are in the process of developing probably the first multi-dimensional, deformable, geothermal reservoir model.[21-23] They have constructed and tested separate two-phase fluid-heat flow and deformation models, and presently are in the process of coupling these. The multi-dimensional deformation model is designed to make possible the use of a variety of elastic and/or plastic constitutive relations. They plan first to apply the model to the Wairakei geothermal field in New Zealand, and wish thereafter to apply it to a site in the Imperial Valley of California.

Lippmann and Narasimhan are presently working to incorporate heat drive and temperature dependencies into the formerly described isothermal groundwater model of Narasimhan.[13] The resulting model will be a one-phase, three-dimensional geothermal reservoir flow model, combined with a one-dimensional deformation model based on the Terzaghi consolidation theory. It will therefore be unable to simulate horizontal ground movements.

Safai and Pinder are presently developing a single-phase, two-dimensional axi-symmetric geothermal deformation model. For this, Biot's three-dimensional elastic theory is being extended to a three-dimensional visco-elastic theory in such a way that the elastic part can be weighted to control the amount of deformation irreversibility obtained.

Discussion and Conclusions

We have discussed subsidence models in three categories: simplified models, advanced subsidence models, and the state-of-the-art.

The status of the current modeling efforts may be summarized as follows: at least ten subsidence models have been developed for pore-fluid withdrawal, and another five are known to be under development with three nearing completion. Firm plans for at least four more are known to the authors.

Compared with the requirements of an advanced subsidence model, the present status of subsidence modeling is seen to be in its infancy. With regard to spatial coverage, one-and two-dimentional capabilities are most common in the current modeling efforts; the few three-dimensional capabilities have, as yet, been little tested. With regard to mechanical properties of reservoir materials, most of the earlier models employed elastic deformation or Terzaghi's one-dimensional consolidation theory. More recently a few have provided a capability for deformation irreversibility by incorporating two different elastic coefficients, a larger one for compaction and a smaller one for expansion. Development of models employing plasticity is just beginning.

With regard to numerical methods, finite difference methods have generally been employed in the flow models, and finite element methods in the deformation models. There are, of course, a few variations upon this theme.

The need for further work is evident from a comparison of the above discussion and the previously stated requirements for an advanced model. The most challenging problem lies in the modeling of the rheological behavior (deformation properties) of the geological materials. A second problem lies in determining the best way to model the reservoir flow-reservoir compaction interaction. Overall, there are also several difficult problems of numerical analysis in reducing the run time of multi-dimensional simulators to an acceptable level.

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UNSTEADY-STATE, MULTI-DIMENSIONAL ANALYTICAL MODELING OF WATER QUALITY IN RIVERS

Robert W. Cleary
Water Resources Program
Princeton University
Princeton, New Jersey

Summary

The unsteady-state, two-and three-dimensional, convective-dispersive mass transport partial differential equations which describe the concentration distribution of a contaminant released as a line, point or general source have been solved analytically using integral transform methods. General two-and three-dimensional modular solutions are presented in closed-form which may be used to obtain the exact solution to a variety of particular boundary conditions and source/sink formulations. Several exact solutions for unsteady-state, two and three-dimensional water quality problems subject to finite geometry boundary conditions are derived from these modular solutions and presented in closed form.

The solutions may be used to model many water quality variables including: BOD, temperature, chlorides, and dye tracers. They are in the form of rapidly-converging infinite series and error functions and are easily and inexpensively applied. In addition to their value as simulation tools, these closed-form expressions may be used to verify multi-dimensional, digital computer numerical models which in many cases could not previously be independently checked.

Introduction

In recent years the modeling of water quality in rivers has advanced from simple one-dimensional analyses to the more accurate and also more complicated two-and three dimentsional approaches.[1,2,3,4,5,6,7] In general, most of the multi-dimensional models presented in the literature have been solved by numerical techniques. Analytical solutions in two and three dimensions are notably lacking. Those closed-form expressions which are available are generally based on infinite geometry systems and have largely been borrowed from the air pollution literature. Boundary effects have either been ignored or in special cases been accounted for using the method of images. The method of images works well for homogeneous first and second type boundary conditions but for cases of a non-homogeneous boundary concentration (e.g., concentration varies as a function of time) or a boundary flux (e.g., benthic deposits of phosphorus diffuse into overlying waters), the method fails.

Despite the wide availability of numerical models for multi-dimensional water quality problems, it is the opinion of the author that a need exists for analytical models. In a given water quality situation the selected model should be commensurate with the questions being asked. Very often these questions can be answered by a closed-form analytical model without resorting to the complexities, computation problems, and expenses of a large numerical mode. To be sure, the analytical model often requires coefficients to be average constants while the numerical model is more flexible, allowing for coefficients to vary throughout time and space. However, in most field situations one does not know how these coefficients vary spatially and the numerical modeler often must use average constants over a given large region. Numerical models are also often plagued by maladies inherent in approximating derivatives by numerical analogs. The most serious of these are numerical dispersion (in cases of convective flows), stability and convergence. Anyone who has worked with numerical models can appreciate the unbelievable frustrations these digital computer maladies can give. It is particularly bothersome when the digital program is extremely large (over a few thousand cards) and one is trying to track down the bug which is causing the program to blow up when a different range of a parameter is used. Numerical models may often require large memories which may only be available on certain computers. Or they may require inordinate amounts of time to complete a simulation and are thus expensive to operate over a long period of real time. They also require skilled operators to set-up, run, and interpret the output. This may preclude their use by small consulting companies or public agencies with limited budgets.

It is the opinion of the author that in many cases, if one considers the questions being asked, the expense and complexities of applying a numerical model, and the ease of applying an analytical expression, one will opt for the analytical solution and will find it adequate for estimating the expected water quality under the given circumstances.

Multi-Dimensional Analytical Solutions

It has been noted that multi-dimensional analytical solutions to the convective-dispersive transport equation for rivers with finite depths and widths are significantly absent in the literature. There are many solutions to the straight diffusion equation.[8] However, modifying this equation to account for convective fluid motion complicates its analytical solution. Additional complications are also introduced by the presence of boundaries, in that the final analytical expression must satisfy the operating boundary conditions. If these boundary conditions are non-homogeneous functions of space and time, the problem is immensely complex, when standard methods are used.

The purpose of this paper is to present the solution technique and analytical solutions to the two-and three-dimensional, unsteady-state, non-homogeneous convective-dispersive, general transport equations which describe the spatial and temporal distribution of a water quality variable in a river. The solution technique is a systematic integral transform approach which easily handles non-homogeneous source/sink terms and non-homogeneous boundary conditions which are functions of space and/or time.

The River Coordinate System

The river is modeled by rectangular geometry as shown in Figure 1. The average width of the river is W, the average height is H, and the flow is predominantly in the longitudinal direction and is described by the cross-sectionally, time-averaged constant velocity U.

Water Quality Transport Equation

Multi-dimensional river water quality is mathematically described by the convective-dispersive transport equation modified for general source/sink activity. This equation may be written in vector notation as follows:

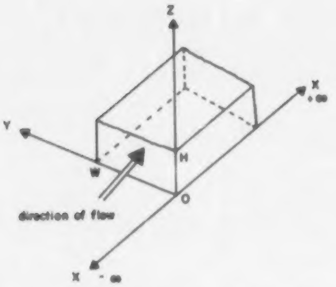

Figure 1. River Coordinate System

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial X} = \nabla(D \cdot \nabla C) \pm G \tag{1}$$

where C represents the concentration of a given water quality variable, U is a constant, averaged velocity, D represents effective dispersion coefficients in the appropriate dimensions, t represents time and G represents a non-homogeneous source or sink function. In the case of first order biological decay in the river, one would add -KC to the right-hand side of equation (1). We will not carry such a modification through our analyses, as the final results are easily modified to account for such decay. It should be noted at this point that the assumptions of constant velocity and constant (but numerically different) effective dispersion coefficients place important limitations on the solutions. Velocity can vary spatially in a river and there is some evidence that the vertical dispersion coefficient may have a parabolic distribution.[9] Notwithstanding these limitations, the solutions represent a significant improvement over present "boundary-less" solutions (which also assume a constant, averaged velocity and constant dispersion coefficients). They also are commensurate with many of the questions being asked by decisionmakers and in cases where a numerical model must be used, they can serve as an important and necessary check on the accuracy of the numerical scheme, for the particular case of constant coefficients.

General Two-Dimensional Solution

In two dimensions, equation (1) reduces to:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial X} = D_x\frac{\partial^2 C}{\partial X^2} + D_z\frac{\partial^2 C}{\partial Z^2} \pm \hat{G}(X,Z,t) \tag{2}$$

To maintain complete generality, equation (2) will be solved subject to non-homogeneous third type boundary conditions. In this way, first type (concentration specified) and second type (flux specified) boundary conditions are automatically included in the final solution. A general non-homogeneous initial condition as well as an arbitrary source/sink function will also be used. Under such specifications, the final solution will be modular in form and can be used to solve a host of non-homogeneous boundary value problems of the first, second, or third type with non-homogeneous generation or depletion. The boundary and initial conditions are:

$$-D_z\frac{\partial C}{\partial Z} + h_3 C = \hat{f}_3(X,t) \qquad Z = 0 \tag{2a}$$

$$D_z\frac{\partial C}{\partial Z} + h_4 C = \hat{f}_4(X,t) \qquad Z = H \tag{2b}$$

$$C \longrightarrow 0 \qquad X \longrightarrow \pm\infty \tag{2c}$$

$$C = F(X,Z) \qquad t = 0 \tag{2d}$$

If C does not approach zero as X approaches infinity, but instead approaches a predictable constant value, one may define a new variable which represents the concentration in excess of this constant value. An example source term, G (X,Z,t), might be a line source, which would describe the release of a contaminant from a diffuser pipe. An instantaneous release would be modeled by three Dirac delta functions:

$$G_L = g_L^i\,\delta(X-X_1)\,\delta(Z-Z_1)\,\delta(t-t_o) \tag{3}$$

where g_L^i represents the instantaneous line source strength (e.g., grams/foot of stream width), X_1 is the longitudinal source location, and Z_1 is the vertical source location; t_o is the time of release.

Equation (2) and associated initial and boundary conditions may be further simplified by introducing the following dimensionless variables:

$$\eta = \frac{XU}{D_x} \qquad \xi = \frac{Z}{H} \qquad \tau = \frac{U^2 t}{D_x} \qquad \zeta = \eta - \tau$$

$$P_2 = \frac{U^2H^2}{D_xD_z} \qquad G = \frac{\hat{G}D_x}{U^2} \qquad f_3 = \frac{\hat{f}_3H}{D_z} \qquad H_3 = \frac{h_3H}{D_z}$$

$$f_4 = \frac{\hat{f}_4H}{D_z} \qquad H_4 = \frac{h_4H}{D_z} \tag{4}$$

Introducing these variables into equation (2) results in a straight diffusion equation:

$$\frac{\partial C}{\partial \tau} = \frac{\partial^2 C}{\partial \zeta^2} + \frac{1}{P_2}\frac{\partial^2 C}{\partial \xi^2} \pm G(\zeta,\xi,\tau) \tag{5}$$

subject to the following dimensionless initial and boundary conditions:

$$-\frac{\partial C}{\partial \xi} + H_3C = f_3(\zeta,\tau) \qquad \xi = 0 \tag{5a}$$

$$\frac{\partial C}{\partial \xi} + H_4C = f_4(\zeta,\tau) \qquad \xi = 1 \tag{5b}$$

$$C \longrightarrow 0 \qquad \zeta \longrightarrow \pm\infty \tag{5c}$$

$$C = F(\zeta,\xi) \qquad \tau = 0 \tag{5d}$$

Method of Solution

If one attempts to solve equation (5) by the common separation of variables method, severe difficulties are encountered due to the spatial and temporal non-homogeneities introduced by the functions: G, f_3 and f_4. After separation of variables, the resulting equation in the finite space variable does not meet Sturm-Liouville requirements for the equation or boundary conditions. Such problems may explain the notable lack of analytical solutions for multidimensional, non-homogeneous, partial differential equations in the literature. One of the purposes of this paper is to illustrate a general integral transform solution technique which may be used to solve problems like equation (5), regardless of how non-homogeneous they are. The ease with which the technique handles spatial and temporal non-homogeneities makes such an approach very powerful and useful in modeling water quality in rivers. Indeed, the methods may be used to solve a host of urresolved problems in many areas of environmental and water resources engineering.

To avoid keeping the analysis too esoteric, more details of the solution method will be presented than is customary. Essentially the method is based on integrally transforming all spatial derivatives out of the equation, leaving only an ordinary differential equation in time. This equation is solved directly and the transformed water quality variable is then inverted back by previously defined inversion formulas to obtain the desired solution. In Cartesian coordinates, the usual integral transforms will be the Fourier (semi-infinite space variables), complex Fourier (infinite) and Finite Fourier (finite). Considering only first (Dirichlet), second (Neumann) and third (Robin or mixed) type boundary conditions, there are three possible kernels for the Fourier transform and nine possible kernels for the Finite Fourier transform. The appropriate kernel to use depends, of course, on the type of boundary conditions present. In the case of the Finite Fourier transform, there are also nine associated eigenvalue relationships. The kernels and associated eigenvalue expressions come from solving the homogeneous analogs of the original, variable-separated partial differential equation. Since the kernels depend only on the type of boundary condition present, once they have been tabulated, they can be used in a variety of different water quality problems for which the only similarity is the type (first, second, or third) of boundary conditions present (the particular non-homogeneous function associated with each type boundary condition does not affect the analytical form of the kernel: it is only the type itself which is important).

Equation (5) has one finite (vertical) and one infinite (longitudinal) dimension. These space variables may be transformed out of the equation by a Finite Fourier and a complex Fourier transform, respectively. The result will be an ordinary differential equation in time, which may be integrated directly for the transformed concentration variable. This transformed variable is then inverted twice by previously defined inversion formulas to yield the solution to equation (5).

To remove the two space variables the following double integral transform and corresponding double inversion formula[10,11,12] for the concentration function $C(\zeta,\xi,\tau)$ in the ranges: $-\infty<\zeta<\infty$, $0\leq\xi\leq 1$ are defined:

$$\overline{\overline{C}}(\beta,\nu_N,\tau) = \int_{-\infty}^{\infty} \exp(i\beta\zeta') \int_0^1 K(\nu_N,\xi')\ C(\zeta',\xi',\tau)d\xi'd\zeta' \tag{6}$$

$$C(\zeta,\xi,\tau) = \frac{1}{2\pi} \sum_{N=0}^{\infty} K(\nu_N,\xi) \int_{-\infty}^{\infty} \exp(-i\beta\zeta)\ \overline{\overline{C}}(\beta,\nu_N,\tau)d\beta \tag{7}$$

where $i = (-1)^{1/2}$ and ν_N are eigenvalues. The transform kernel, $K(\nu_N,\xi)$, is the normalized eigenfunction of the following associated eigenvalue problem:

$$\frac{d^2V(\xi)}{d\xi^2} + \nu^2\ V(\xi) = 0 \tag{8}$$

subject to:

$$-\frac{dV(\xi)}{d\xi} + H_3\ V(\xi) = 0 \qquad \xi = 0 \tag{8a}$$

$$\frac{dV}{d\xi} + H_4\ V(\xi) = 0 \qquad \xi = 1 \tag{8b}$$

This eigenvalue problem comes from separating the variables of the original partial differential equation. Multiplying equation (5) by $K(\nu_N,\xi')\exp(i\beta\zeta')$ and integrating over ζ' and ξ' from $-\infty$ to ∞ and 0 to 1, respectively, the following is obtained:

$$\frac{d\overline{\overline{C}}}{d\tau} = -\beta^2\overline{\overline{C}} + \frac{1}{P_2}\left[-\nu_N^2\overline{\overline{C}} + K(\nu_N,\xi)\Big|_{\xi=0}\int_{-\infty}^{\infty} f_3\exp(i\beta\zeta')d\zeta' + K(\nu_N,\xi)\Big|_{\xi=1}\int_{-\infty}^{\infty} f_4\exp(i\beta\zeta')d\zeta'\right] + \overline{\overline{G}}(\beta,\nu_N,\tau) \tag{9}$$

subject to the initial condition:

$$\overline{\overline{C}} = \int_0^1 K(\nu_N,\xi')\int_{-\infty}^{\infty} F(\zeta',\xi')\exp(i\beta\zeta')d\zeta'd\xi' \qquad \tau = 0 \tag{9a}$$

The bars indicate transformed variables according to the definition given by equation (6). Equation (9) is a non-homogeneous, first order ordinary differential equation for which there is an integrating factor. The direct integration of equation (9) gives an expression for the double-transformed concentration variable. This expression is substituted into the double inversion given by equation (7) and after rearrangement, the final solution to equation (5) is:

$$C(\zeta,\xi,\tau) = \frac{1}{2\pi}\sum_{N=0}^{\infty} K(\nu_N,\xi)\int_{-\infty}^{\infty} \exp(-i\beta\zeta-\mu\tau)[\overline{\overline{F}}(\beta,\nu_N) + \int_0^{\tau}\exp(\mu\tau')\cdot A(\beta,\nu_N,\tau')d\tau']d\beta \tag{10}$$

where

$$A(\beta,\nu_N,\tau') = \int_0^1 K(\nu_N,\xi')\int_{-\infty}^{\infty} G(\zeta';\xi';\tau')\exp(i\beta\zeta')d\zeta'd\xi' + \frac{1}{P_2}\left[K(\nu_N,\xi)\Big|_{\xi=0}\int_{-\infty}^{\infty} f_3(\zeta',\tau')\exp(i\beta\zeta')d\zeta' + K(\nu_N,\xi)\Big|_{\xi=1}\int_{-\infty}^{\infty} f_4(\zeta',\tau')\exp(i\beta\zeta')d\zeta'\right]$$

$$\mu = \beta^2 + \frac{\nu_N^2}{P_2} \tag{10a}$$

and:

$$\overline{\overline{F}}(\beta,\nu_N) = \int_0^1 K(\nu_N,\xi')\int_{-\infty}^{\infty} F(\zeta';\xi')\exp(i\beta\zeta')d\zeta'd\xi' \tag{10b}$$

Equation (10) is the general, analytical, modular solution to the dimensionless, two-dimensional, water quality transport equation for rivers. It can account for non-homogeneous generation/depletion and non-homogeneous first, second or third type boundary conditions. In the special case of a first type boundary condition at either $\xi = 0$ or $\xi = 1$, one modified the kernel evaluated at the point in equation (10a) by replacing:

$$K(\nu_N,\xi)\Big|_{\xi=0} \quad \text{by} \quad \frac{dK(\nu_N,\xi)}{d\xi}\Big|_{\xi=0} \tag{11}$$

or

$$K(\nu_N,\xi)\Big|_{\xi=1} \quad \text{by} \quad -\frac{dK(\nu_N,\xi)}{d\xi}\Big|_{\xi=1} \tag{11a}$$

To use solution (10), one simply substitutes into the total expression his particular G, F, f_3, f_4 and appropriate kernels and carries out the indicated integrations.

General Three-Dimensional Solution

In three dimensions, equation (1) becomes:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial X} = D_x\frac{\partial^2 C}{\partial X^2} + D_y\frac{\partial^2 C}{\partial Y^2} + D_z\frac{\partial^2 C}{\partial Z^2} \pm \hat{G}(X,Y,Z,t) \tag{12}$$

Once again, to maintain complete generality, only third type boundary conditions will be used:

$$-D_z\frac{\partial C}{\partial Z} + h_3C = \hat{f}_3(X,Y,t) \qquad Z = 0 \tag{12a}$$

$$D_z\frac{\partial C}{\partial Z} + h_4C = \hat{f}_4(X,Y,t) \qquad Z = H \tag{12b}$$

$$-D_y\frac{\partial C}{\partial Y} + h_5C = \hat{f}_5(Z,X,t) \qquad Y = 0 \tag{12c}$$

$$D_y\frac{\partial C}{\partial Y} + h_6C = \hat{f}_6(Z,X,t) \qquad Y = W \tag{12d}$$

$$C \longrightarrow 0 \qquad X \longrightarrow \pm\infty \tag{12e}$$

$$C = F(X,Y,Z) \qquad t = 0 \tag{12f}$$

The dimensionless variables given by equations (4) as well as the following additional variables will be incorporated into equation (12) to further generalize it:

$$\zeta = \frac{Y}{W} \qquad P_1 = \frac{U^2W^2}{D_xD_y} \qquad \varepsilon = \eta - \tau \qquad f_5 = \frac{\hat{f}_5W}{D_y}$$

$$H_5 = \frac{h_5W}{D_y} \qquad f_6 = \frac{\hat{f}_6W}{D_y} \qquad H_6 = \frac{h_6W}{D_y} \tag{13}$$

Equation (12) then becomes a straight diffusion equation:

$$\frac{\partial C}{\partial \tau} = \frac{\partial^2 C}{\partial \varepsilon^2} + \frac{1}{P_1}\frac{\partial^2 C}{\partial \zeta^2} + \frac{1}{P_2}\frac{\partial^2 C}{\partial \xi^2} \pm G(\varepsilon,\zeta,\xi,\tau) \tag{14}$$

subject to:

$$-\frac{\partial C}{\partial \zeta} + H_5C = f_5(\xi,\varepsilon,\tau) \qquad \zeta = 0 \tag{14a}$$

$$\frac{\partial C}{\partial \zeta} + H_6C = f_6(\xi,\varepsilon,\tau) \qquad \zeta = 1 \tag{14b}$$

$$-\frac{\partial C}{\partial \xi} + H_3C = f_3(\varepsilon,\zeta,\tau) \qquad \xi = 0 \tag{14c}$$

$$\frac{\partial C}{\partial \xi} + H_4C = f_4(\varepsilon,\zeta,\tau) \qquad \xi = 1 \tag{14d}$$

$$C \longrightarrow 0 \qquad \varepsilon \longrightarrow \pm\infty \tag{14e}$$

$$C = F(\varepsilon,\zeta,\xi) \qquad \tau = 0 \tag{14f}$$

To remove all three space variables, we define a triple integral transform and corresponding triple inversion formula:

$$\bar{\bar{C}}(\phi,\beta_m,\nu_N,\tau) = \int_{-\infty}^{\infty}\int_0^1\int_0^1 \exp(i\phi\varepsilon')K(\beta_m,\zeta')K(\nu_N,\xi') \cdot C(\varepsilon',\zeta',\xi',\tau)d\zeta'd\xi'd\varepsilon' \tag{15}$$

$$C(\varepsilon,\zeta,\xi,\tau) = \frac{1}{2\pi}\sum_{m=0}^{\infty}\sum_{N=0}^{\infty}\int_{-\infty}^{\infty} \exp(-i\phi\varepsilon)K(\beta_m,\zeta)K(\nu_N,\xi) \cdot \bar{\bar{C}}(\phi,\beta_m,\nu_N,\tau)d\phi \tag{16}$$

As in the two-dimensional case, the integral transform defined by equation (15) is applied to equation (14) and its associated initial and boundary conditions. The resulting ordinary differential equation is integrated to obtain the triple-transformed concentration variable which is inverted by equation (16) to yield the following general modular solution:

$$C = \sum_{m=0}^{\infty}\sum_{N=0}^{\infty} K(\beta_m,\zeta)K(\nu_N,\xi)\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(-i\phi\varepsilon)\exp(-\mu\tau) \cdot \left(\bar{\bar{F}}(\phi,\beta_m,\nu_N) + \int_0^{\tau} \exp(\mu\tau')P(\phi,\beta_m,\nu_N,\tau')d\tau'\right)d\phi \tag{17}$$

where:

$$\mu = \phi^2 + \frac{\beta_m^2}{P_1} + \frac{\nu_N^2}{P_2} \tag{17a}$$

and:

$$\begin{aligned} P(\phi,\beta_m,\nu_N,\tau') = {} & \int_{-\infty}^{\infty}\int_0^1\int_0^1 \exp(i\phi\varepsilon')K(\beta_m,\zeta')K(\nu_N,\xi') \\ & \cdot G\, d\varepsilon'd\zeta'd\xi' + \frac{1}{P_1}\Bigg(K(\beta_m,\zeta)\Big|_{\zeta=0} \\ & \cdot \int_{-\infty}^{\infty}\int_0^1 \exp(i\phi\varepsilon')K(\nu_N,\xi') \cdot f_5 d\varepsilon'd\xi' \\ & + K(\beta_m,\zeta)\Big|_{\zeta=1}\int_{-\infty}^{\infty}\int_0^1 \exp(i\phi\varepsilon')K(\nu_N,\xi') \\ & \cdot f_6 d\varepsilon'd\xi'\Bigg) + \frac{1}{P_2}\Bigg(K(\nu_N,\xi)\Big|_{\xi=0} \\ & \cdot \int_{-\infty}^{\infty}\int_0^1 \exp(i\phi\varepsilon')K(\beta_m,\zeta')f_3(\varepsilon',\zeta'\tau)d\varepsilon'd\zeta' \\ & + K(\nu_N,\xi)\Big|_{\xi=1}\int_{-\infty}^{\infty}\int_0^1 \exp(i\phi\varepsilon')K(\beta_m,\zeta') \\ & \cdot f_4 d\varepsilon'd\zeta'\Bigg) \end{aligned} \tag{17b}$$

and

$$\bar{\bar{F}} = \int_{-\infty}^{\infty}\int_0^1\int_0^1 \exp(i\phi\varepsilon')K(\beta_m,\zeta')K(\nu_N,\xi')F\, d\varepsilon'd\zeta'd\xi' \tag{17c}$$

Applications

To illustrate the comprehensive flexibility built into the modular solutions given by equations (10) and (17), selected closed-form solutions, based on these general equations, will be presented. Due to space limitations typical solution details cannot be presented here but may be found elsewhere.[3,6,13]

Two-Dimensional, Instantaneous Tracer Line Source

For this case, the two-dimensional transport equation is subject to a Dirac delta instantaneous line source function and two second type, no-flux boundary conditions at $Z = 0$ and $Z = H$. The details are given in (G). Applying modular solution (10), the solution with dimensions is:

$$C(X,Z,t) = \frac{g_L^1 \exp\left[-\frac{(X-X_1-Ut)^2}{4\,D_x t}\right]}{H(4\pi D_x t)^{1/2}}\left[1+2\sum_{N=1}^{\infty}\exp(-D_z\mu_N^2 t)\cos\mu_N Z\cos\mu_N Z_1\right] \tag{18}$$

Three-Dimensional, Instantaneous Tracer Point Source

In this case, the three-dimensional transport equation is subject to an instantaneous Dirac delta point source function and four second type no-flux boundary conditions at Z=0, Z=H, Y=0, and Y=W. The details may be found in Reference 6. Applying modular solution Equation 17, the solution with dimensions is:

$$C(X,Y,Z,t) = \frac{g_{PT}^1 \exp\left[-\frac{(X-X_1-Ut)^2}{4D_x t}\right]}{WH(4\pi D_x t)^{1/2}} \cdot\left[1+2\sum_{N=1}^{\infty}\exp(-\mu_N^2 D_z t)\cos\mu_N Z\cos\mu_N Z_1\right] \cdot\left[1+2\sum_{m=1}^{\infty}\exp(-\beta_m^2 D_y t)\cos\beta_m Y\cos\beta_m Y_1\right] \tag{19}$$

Three-Dimensional, Biochemical Oxygen Demand Transport

The unsteady-state, three-dimensional, first order decay, transport model for BOD in rivers is given by:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial X} = D_x\frac{\partial^2 C}{\partial X^2} + D_y\frac{\partial^2 C}{\partial Y^2} + D_z\frac{\partial^2 C}{\partial Z^2} - KC + g_{PT}\,\delta(X-X_1)\delta(Y-Y_1)\delta(Z-Z_1) \tag{20}$$

The BOD is released as a continuous point source and is subject to no-flux conditions on all four boundaries. Initially there is zero BOD. The solution may easily be obtained by using equation (17) to derive the solution to the first order decay, instantaneous point source case (similar to equation (19)) and then integrating this solution over time to obtain the continuous point source solution with dimensions:

$$\begin{aligned}
C = {} & \frac{g_{PT}\,\mathrm{EXP}(XU/2D_x)}{4\,W\,H\,(D_x)^{1/2}}\Bigg[\frac{\mathrm{ERFC}(X/(4D_x t)^{1/2}-(k_2 t)^{1/2})}{(k_2)^{1/2}} \\
& \cdot \mathrm{EXP}(-X(k_2/D_x)^{1/2}) - \frac{\mathrm{ERFC}((k_2 t)^{1/2}+X/(4D_x t)^{1/2})}{(k_2)^{1/2}} \\
& \cdot \mathrm{EXP}(X(k_2/D_x)^{1/2}) + 2\sum_{N=1}^{\infty}\frac{\mathrm{COS}\mu_N Z\,\mathrm{COS}\mu_N Z_1}{(k_3)^{1/2}} \\
& \Big(\mathrm{EXP}(-X(k_3/D_x)^{1/2})\mathrm{ERFC}(X/(4D_x t)^{1/2}-(k_3 t)^{1/2}) \\
& - \mathrm{EXP}(X(k_3/D_x)^{1/2})\mathrm{ERFC}((k_3 t)^{1/2}+X/(4D_x t)^{1/2})\Big) \\
& + 2\sum_{m=1}^{\infty}\frac{\mathrm{COS}\beta_m Y\,\mathrm{COS}\beta_m Y_1}{(k_4)^{1/2}}\Big(\mathrm{EXP}(-X(k_4/D_x)^{1/2}) \\
& \cdot \mathrm{ERFC}(X/(4D_x t)^{1/2}-(k_4 t)^{1/2}) \\
& - \mathrm{EXP}(X(k_4/D_x)^{1/2})\mathrm{ERFC}((k_4 t)^{1/2}+X/(4D_x t)^{1/2})\Big) \\
& + 4\sum_{N=1}^{\infty}\sum_{m=1}^{\infty}\frac{\mathrm{COS}\mu_N Z\,\mathrm{COS}\mu_N Z_1\,\mathrm{COS}\beta_m Y\,\mathrm{COS}\beta_m Y_1}{(k_5)^{1/2}} \\
& \cdot\Big(\mathrm{EXP}(-X(k_5/D_x)^{1/2})\mathrm{ERFC}(X/(4D_x t)^{1/2}-(k_5 t)^{1/2}) \\
& - \mathrm{EXP}(X(k_5/D_x)^{1/2})\mathrm{ERFC}((k_5 t)^{1/2}+X/(4D_x t)^{1/2})\Big)\Bigg]
\end{aligned} \tag{21}$$

where:

$k_2 = (U^2/4D_x) + K$; $k_4 = k_2 + \beta_m^2 D_y$; $\mu_N = \frac{N\pi}{H}$; $\beta_m = \frac{m\pi}{W}$

$k_3 = k_2 + \mu_N^2 D_z$; $k_5 = k_2 + \mu_N^2 D_z + \beta_m^2 D_y$

and

$X_1 = 0$; $X > 0$

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SIMULATION MODELING OF ENVIRONMENTAL INTERACTION EFFECTS

Ethan T. Smith
Program Analyst
2014 Golf Course Drive
Reston, Virginia

Abstract

The present research addresses the air-water-land problem simultaneously by means of a series of mathematical models. A steady-state water quality model is used to simulate the effect of biochemical oxygen demanding wastes on the dissolved oxygen concentrations in an estuarine system. A Gaussian plume air quality model is similarly utilized to relate the particulate and sulfur oxide emissions of waste sources to the concentration of these contaminants in the regional airshed. A materials balance model is formulated which simulates the impact of pollution control for a given medium in exacerbating environmental pollution in another medium. A strategy model is formulated that derives removal percentages for air loads and waste water discharges, while simultaneously minimizing the flows of material to solid waste disposal. The constraints on the optimizing strategy model are given by equations which require that ambient quality standards must be attained for dissolved oxygen, particulates, and sulfur oxides.

The set of models is applied to an eleven-county study area centering on the city of Philadelphia, Pa. The results of applying the models indicate that present ambient quality standards can be achieved.

Planning for Environmental Resource Management

The management of the environment, like any activity undertaken by man, requires some method of approach which can be thought of as a plan. On the one hand, this may refer to some rather formal approach involving a sequence of steps arranged in time to achieve some objective. In the absence of a formal approach, actions can still be undertaken which, by default, will tend to be rather independent of one another. In either case, effort will be expended on some mixture of data collection, analysis, negotiation, and modification of the physical world.

A pervasive problem is associated with the nature of cause-effect linkages, or causal chains. The name is perhaps somewhat of a misnomer, since cause-effect interactions related to the environment are seldom simple one or two step processes. Indeed, a much more accurate picture would be that of a multi-branched tree or network structure with numerous feedback loops. Under these circumstances even well-conceived scientific approaches to pollution control have encountered severe problems.

It is now possible to discern the essential characteristics of many environmental problems. Attempts to address these problems often fall into the error of suboptimization. Under these circumstances, solutions may be successful to a greater or lesser degree in dealing with the matter immediately at hand (e.g., Biochemical Oxygen Demand, or BOD, in the water). More relevant however is the fact that secondary effects resulting from the initial solution act to exacerbate other environmental problems, or even to cause new problems.

The concept of materials balance appears to offer a promising route toward the resolution of these kinds of difficulties.[1] In this approach, the principle of conservation of mass is applied to material goods as they pass through the system, undergoing of course many changes in form. If successful, this kind of analysis should identify the residual materials that are byproduct from the processing steps which are designed to yield the economic products of society. This makes it possible at least in principle to specify the links in the causal network in quantitative terms. This study is focused on just a small part of the general materials balance model, specifically the routing available to control some of the major contaminants of air, water, and land.

Even in the present rather modest form, this work significantly transcends traditional concepts of pollution control, and is perhaps best described as resource management. This process begins to explore the tradeoffs possible among (a) the level of technology, (b) the spatial needs for land use, (c) the concentration of contaminants in the ambient environment. There are also important implications for the use of natural resources such as water and fisheries for many purposes (e.g., recreation), and at a further remove, the use of mineral and energy resources required to achieve pollution control by technology. Ultimately, this type of research is capable of contributing to a definition in quantitative terms of the carrying capacity of regions for human activity.[2]

First, it is important to include secondary effects within the set of decisions variables. Thus, to take one example, the increase of treatment which removes BOD from wastewater must be reflected as some combination of routing to land and air. Organic sludge either is sent to a disposal site or is incinerated, and in the latter case it acts to lower air quality. The incineration can be accomplished either on site or at a municipal incinerator. Simultaneously, controls applied to industrial stacks will result in either ash to be sent to a landfill (if dry removed) or solids in the sewerage system (if wet scrubbed). At least some part of these solids will be removed at a sewage treatment plant and will cycle through the system. Second, the foregoing description, when applied to a large number of treatment plants, firms, incinerators, power plants, and landfills, leads to complicated spatial interaction as materials are routed from point to point. This is especially true in a relatively large region like the present eleven county study area encompassing the Trenton-Philadelphia-Wilmington SMSA's. Superimposed on this interaction is a requirement for segregating political jurisdictions and accounting for physical barriers which would preclude particular paths in a real case. Next, there is a requirement for state-of-the-art air and water quality dispersion models with the best possible validation procedures. Without field-testing, there is small probability that conclusions reached by these models will be acceptable. In order to accomplish these objectives, the following residuals control and routing processes have been analyzed:

a. Treatment at sewage treatment plants (STP's),
b. Treatment at firms possessing individual wastewater facilities,
c. Control of particulates and SO_2 at individual STP's, firms, power plants, and municipal incinerators,
d. Control of particulates and SO_2 by area sources,
e. Routing of area source solid waste to land disposal,
f. Routing of sludge from STP's and firms to municipal incinerators,
g. Routing of wet scrubbed particulates and SO_2 to sewerage system, STP's and river,
h. Routing of sludge from STP's and firms to land disposal,
i. Routing of dry removed particulates and SO_2 to land disposal.

These processes are shown in Table 1. To facilitate modeling these processes, a series of decision variables is defined, which are common to each process. These decision variables are as follows:

D_w = BOD allocated to the water,

D_a = BOD allocated (in transformed form) to the air, by incineration of sludge solids,

D_s = BOD allocated to solid waste disposal, as removed sludge solids,

E_a = Particulates allocated to the air,

E_w = Particulates allocated to the water, by wet scrubbing,

E_s = Particulates allocated to solid waste disposal, by dry removal,

F_a = SO_2 allocated to the air,

F_w = SO_2 allocated to the water, by wet scrubbing with limestone,

F_s = SO_2 allocated to solid waste disposal, by dry removal with limestone.

These decision variables act to allocate the various residual streams among three possible media: air, water, and land. The variables are applied in each of the control and routing processes, at the completion of which the total residuals discharged to the media as a result of these processes are obtained. All allocation variables are in terms of percentages of untreated (or raw) waste load, and hence are dimensionless. It is essential to realize that all percentages for a given residual sum to one, i.e., $D_w + D_a + D_s = 1.0$. The allocation variables are readily related to familiar quantities: for example, the percent removal of BOD at a wastewater treatment plant is $1.0 - D_w$. Similarly, the percent reduction of particulates to the air at a specific facility is $1.0 - E_a$. The other allocation variables are defined in parallel manner.

Results of Routing Processes

The results of the routing processes shown in Table 1 can be summarized as follows, with special reference to mass discharged to the air, water, or land as residuals:

Sources (k) which discharge directly to surface water (including STP's), discharge BOD as a function of D_w, as well as solids resulting from the scrubbing of stack gases as a function of E_w and F_w. Particulates and SO_2 are emitted to the air, both from sludge incineration and industrial processes. Land disposal is provided for treatment plant sludge and solids.

Controls are used (E_a and F_a) to reduce the emission of particulates and SO_2 at sources of the industrial (m), municipal incinerator(i), and power plant (j) types. Solids which are scrubbed out are routed to collection systems and to land disposal by E_w, E_s, F_w, and F_s except for sources having access to surface water, such as power plants.

Area sources (n), which cover perhaps five to 25 square miles each, contain a heterogeneous assortment of emissions, often with large contributions from residential and commerical land uses. The space heating and refuse incineration aspects of these sources are included, by allocating part of the solid waste to land disposal. In the case of these sources, it is reasonable to assume that reduction of air emissions occurs through fuel switching and the restriction of local incineration practices.

The routing of materials according to the spatial configuration of the study area requires some assumption for choice among alternative destinations. It is assumed that under long-term average conditions the physically nearest destination will be selected. In reality, service areas are probably better determinants for selection of destinations, e.g., which landfill will service which source; however, such information is usually not readily available. In addition, destinations are required to be in the same political jurisdiction (Del., N.J., Pa., or Philadelphia) as the source being serviced. This constraint adds reality to decisions under consideration, and helps to demonstrate the consequences of such a restriction.

In the case of landfills, the selected site is checked to determine whether the acreage required is available; if not, sites progressively further away are examined until all conditions are met. If no landfill meets all conditions, the unmet demand is recorded as a requirement for further acreage.

Water Quality Model Formulation

A one-dimensional, steady-state, finite-difference model of the Delaware Estuary is employed for the coupled variables BOD-DO. Similar formulations may be found in Thomann[3] who has worked extensively with the coupled-system approach. Figure 1 is a map of the Delaware Estuary showing the 30 segments or sections of the mathematical model. This estuary constitutes the receiving surface water in this study. For each of these model sections a mass-balance equation can be written for the BOD in the system, and another for the DO in the system. This results in linear differential equations based on the physical, hydrologic, and biochemical characteristics of each section.

This model, expressed in matrix form, is:

$$(c) = (c_s) - (c_j) \pm (c_p) \qquad (1)$$

$$(c_j) = (A)(J) \qquad (2)$$

$$(c_p) = (B)(P) \qquad (3)$$

where (c_j) is the Dissolved Oxygen (DO) response in each section to the vector of effluent BOD discharge loads (J), and (A) is the square matrix showing the steady-state DO response in all sections due to a unit BOD discharge in any section. (c_s) is the saturation value of DO in each section. The DO response of the system to an in-place source or sink of oxygen P is expressed in equation 3, which may then be combined with the DO response created by the (J) loads to give the total DO response (c). In practice (P) represents the effects of phenomena like photosynthesis and benthal deposits.

The matrix (A) can be used to evaluate the effect of modifying the discharge BOD loads (J) on the DO profile. If $(\Delta J) = f(D_w)$ represents reducing the discharged effluent load by increasing waste treatment, the increased DO profile can be computed as:

$$(c) = (c_s) - (c_j) \pm (c_p) + (A)(\Delta J). \qquad (4)$$

The model has been verified by the Delaware Estuary Comprehensive Study, based on research conducted from 1961 to 1969.[4] In addition, time-series studies by Thomann make it possible to calculate a variance of about 1.56 mg/l around the summer mean values of DO computed by the model.[5]

Since (ΔJ) is a function of the allocation variable D_w, it is possible to evaluate the DO profile in equation 4 by specifying D_w, and to compare the vector (c) against water quality standards.

Air Quality Model Formulation

Mathematical models of air quality represent a relationship between the sources of air pollution and the result as measured in the ambient air. With the establishment of air quality standards it becomes necessary to employ some such relationship to determine what modification of the source emission loads is required if the ambient standards are to be met.

The atmospheric characteristics are simulated in the mathematical model under specific assumptions. The first of these is that the discharge emitted from each source will take the form of a Gaussian plume. This means that the dispersion of the plume at a distance downwind is assumed to follow a Gaussin distribution in directions perpendicular to the wind vector. The concentration of pollutant can then be calculated by applying a normal probability function. In the form used here this is usually termed the Martin-Tikvart model.[6]

In this case, the model takes the form

$$X_{sr} = \sum_{u}\sum_{v} S_{duv}\, X_s\,(Q_s, x, u, \sigma_z, h) \qquad (5)$$

which shows the ambient concentration X_{sr} at receiving point r due to source s emission of pollutant Q_s. The downwind distance x, wind speed u, vertical atmospheric dispersion σ_z, and source height h are used in the functional form. The joint frequency distribution S_{duv} gives the frequency of occurrence of wind in direction d in speed class u and stability class v. At a given receiving point (receptor) concentrations from all sources are superimposed.

$$X_r = \sum_{s} X_{sr} \qquad (6)$$

The model has been calibrated for the study area by EPA using 1968 data for particulates and SO_2. Regression and correlation yields r values of 0.87 and 0.88, respectively. Variation around the annual average predictions of the model is on the order of ± 15 to 20%.[7]

The source emission Q_s is a function of the allocation variable E_a or F_a, depending on pollutant. Therefore, equation 6 can be evaluated for each receptor point r as function of E_a and F_a, i.e., $X_r = f(E_a, F_a)$. Contour maps of X_r can be compared to ambient air quality standards.

Ambient Quality Data

The initial conditions for the analysis are given by the present state of the system. A part of this state is measured in terms of the numerical values of ambient environmental quality. In the case of water quality, the dissolved oxygen concentrations are based on the work of the Delaware Estuary Comprehensive Study. An initial verification of the water model was carried out for 1964 data. Subsequently, the data were updated to 1968 and to 1970, principally by accounting for the growth of effluent discharges.[4,8,9]

The DO standards and initial DO profile for the Delaware Estuary are given in detail in Figure 6. The DO standards are those of the Delaware River Basin Commission (DRBC).[10]

The data base for particulate and SO_2 concentration is taken from the EPA Implementation Planning Program work on the Philadelphia Air Quality Control Region.[7] The existing air quality in this reference is based on measurements from 1968. Figure 2 shows the 1968 annual average pattern of particulate concentration in the study area, and Figure 3 shows the pattern for SO_2. This data base has been used by EPA to validate the Gaussian plume air quality model used in this study.

The air quality standards sought in this study are an annual geometric mean of 75 ug/m3 for particulates, and an annual arithmetic mean of 80 ug/m3, for sulfur oxides.[11]

Discharge Loads to the Environment

In order to carry out analysis of the study area, numerical measures of the discharges to the environment are necessary. Ideally, the discharge data should be for the same year as the ambient quality date (in this case 1968) so as to permit prediction of improvement in environmental quality as a result of modifying the discharges.

Discharge data for effluents to the Delaware Estuary are available in terms of BOD.[8,9] All values are in terms of first stage carbonaceous BOD discharged at the outfall, for 1968. The present research includes 24 sewage treatment plant effluents, which comprise about 98% of the BOD discharged to the estuary by municipal waste sources. In addition, 29 industrial firms are included which possess wastewater discharges from company-owned treatment facilities. These sources account for about 96% of the BOD discharged to the estuary by industrial waste sources.

Discharge data for air emissions to the study area are available as part of the data base used by EPA in the Implementation Planning Program.[7] For the year of 1968 both particulate and SO_2 emissions exist for each stack in the source data file for the Philadelphia Air Quality Control Region. The following set of air emission sources is input to the model:

a. 58 industrial sources accounting for about 85% of the SO_2 and 84% of the particulates from all such sources,
b. 16 municipal incinerators accounting for about 97% of the SO_2 and 78% of the particulates from all such sources,
c. 10 steam-electric generating plants accounting for about 82% of the SO_2 and 89% of the particulates from all such sources.
d. 55 area sources accounting for about 63% of the SO_2 and 55% of the particulates from all such sources.

The most recent National Survey of Solid Waste Practices is for the year 1968, which makes it possible to obtain landfill data contemporary with the rest of the research.[12] Forty-nine landfills and available acreage at each site (located by Cartesian coordinates) are used in this study.

Strategy Model

There are nine decision variables represented by the allocation variables which divide residuals among water, air, and land. The ambient environmental standards have been specified for both airborne and waterborne contaminants, and models developed to predict changes in ambient concentrations as a function of materials routing. The remaining problem is to determine the values of the decision variables that will enable all quality goals to be satisfied.

Recognizing the possible tradeoffs in the construction of optimization models, the approach selected in this study relies on an assumption that the percent removal of a given material must be equal for all waste sources of one type. This approach has the following characteristics:

a. It is mathematically simpler than a linear or nonlinear programming approach,
b. The assumption of equal percent removal is often administratively favored, even though less flexible than an approach allowing sources to be individually adjusted,
c. It does permit all ambient standards to be achieved simultaneously,
d. Damage (cost) functions are not explicitly represented in the model, although such functions are implicit in the ambient quality standards, since meeting the standards is often taken as equivalent to minimizing damages.

Mathematically, the strategy model can be described as follows:

$$\text{MIN} \left\{ \sum_k V_k(D_s) + \sum_\theta V_\theta(E_s) + \sum_\theta V_\theta(F_s) \right\}, \quad (7)$$

subject to $(A)(\Delta J) \geq (c_g)$ $\quad \theta = i,m,j,n$

where $\quad \Delta J_k = (D_{owk} - D_w)\, T_k$

and $\quad X_r\,(\Delta Q_s) \leq X_{rg}$ for particulates and SO_2

where $\quad \Delta Q_s = (E_{oas} - E_a)\, P_s$ for particulates

$\quad = (F_{oas} - F_a)\, U_s$ for SO_2.

$$D_w + D_a + D_s = 1.0,$$
$$E_w + E_a + E_s = 1.0,$$
$$F_w + F_a + F_s = 1.0.$$

Equation 7 shows the minimization of volumes V of mass allocated to land disposal for all source types; this process is constrained by modification of the ΔJ_k loads so as to meet the incremental DO goal (c_g). D_{owk} is the initial percentage allocated to the water, and T_k is sum of BOD residuals generated. Similarly, modifications of air source emissions ΔQ_s must meet the ambient air standards X_{rg}. This depends on initial percentage allocations E_{oas} and F_{oas} for each source s, and on P_s and U_s, the sum of particulate and SO_2 residuals generated (see Table 1).

Model Results

The derived values of the allocation percentages indicate that 91% Carbonaceous BOD removal is required for all sources discharging into the Delaware Estuary. Similarly, 75% removal of particulates and 72% removal of SO_2 is called for in the case of sources having air emissions. In all cases these are percentages of untreated waste discharges. At this point it should be noted that one result of recent EPA work on this river called for a 50% reduction in Nitrogenous BOD discharges to be superimposed on these conclusions.[9] Other conclusions are that 30% of the sludge produced should be incinerated, and 61% of it consigned to land disposal.

The effect of the treatment levels can be seen in the predicted improvement in the quality of the environment. The resultant dissolved oxygen profile is shown in Figure 6. Except in the three sections containing the "Bristol Sag" (5 through 7) the DO standards for summer average conditions are attained everywhere. The primary annual average air quality standards of 75 ug/m3 for particulates and 80 ug/m3 for SO_2 are also achieved. Figure 4 shows the resultant particulate concentration pattern for the study area. Figure 5 shows the SO_2 pattern resulting from the strategy. These figures clearly show the effect of load reduction in breaking up the region-wide pattern into a few peaks of high concentration which tend to be centered on dense urban and/or industrial sources within the study area.

The routing of residuals to land ultimately results in the consumption of space at the sanitary landfills in the study area. The model will attempt to utilize all available space in accordance with the routing and jurisdiction rules, and will route any remaining solid waste to another category which represents the amount by which demand exceeds supply. The demand excess is as follows:

New Jersey	309 acres
Pennsylvania	239 acres
Philadelphia	739 acres
Delaware	zero

These figures represent demands generated by this study alone, and are in addition to any other acreage requirements.

The significance of this analysis is:

a. Numerous air-water-land interactions can be simulated so as to produce quantitative, non-intuitive results. If desired, ambient standards can be easily altered and sensitivity analysis performed on these and other variables.

b. Numerical results show that required controls are probably within the range of current technology. This implies that changes in land resources; e.g., changes in density, can be avoided or at least postponed.

c. The attainment of water quality standards implies optimum utilization of, e.g., recreation and fisheries resources, as defined by the standards for the region.

d. The emerging problem of solids disposal is quantitatively defined as it would impact land use if land disposal is used.

e. The methodology is transferable to other study areas where discharge loads, ambient air/water quality data, land disposal data, and model parameters are available. Assembling such data should become easier as a result of recent public laws.

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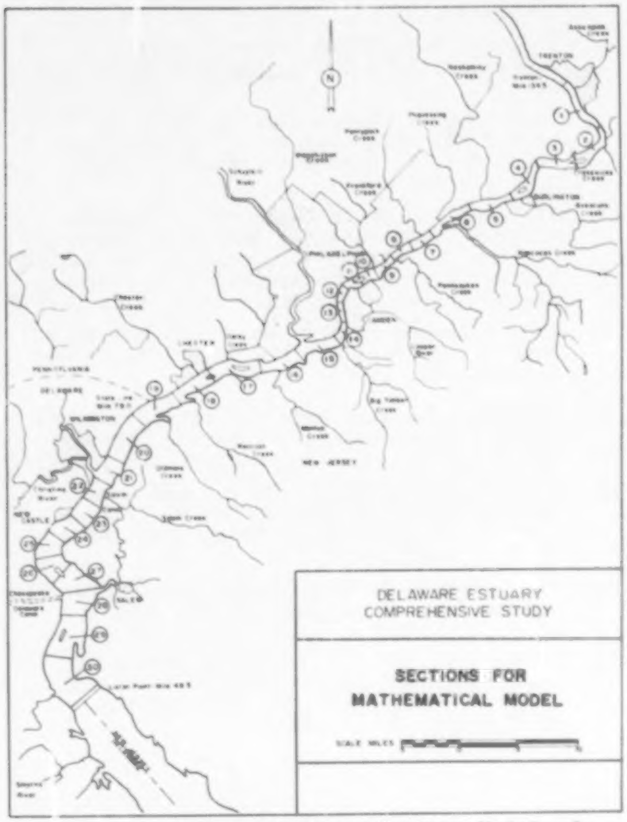
TO FROM	DIRECT-DISCHARGERS (STPs & IND.) k	MUNICIPAL INCINERATORS 1	LAND DISPOSAL 1	AIR	SURFACE WATER
DIRECT-DISCHARGERS (STPs & IND.) k		SLUDGE	SLUDGE, SOLIDS	PARTICULATES, SO_2	BOD, SOLIDS
MUNICIPAL INCINERATORS 1	SOLIDS		SOLIDS	PARTICULATES, SO_2	
INDUSTRIAL SOURCES m	SOLIDS		SOLIDS	PARTICULATES, SO_2	
POWER PLANTS j			SOLIDS	PARTICULATES, SO_2	SOLIDS
AREA SOURCES n			SOLID WASTE	PARTICULATES, SO_2	

Table 1 - Residuals Routing Process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SCALE MILES
TRENTON
BURLINGTON
PHILADELPHIA
CAMDEN
CHESTER
WILMINGTON
NEW CASTLE
SALEM
PENNSYLVANIA
DELAWARE
NEW JERSEY
Schuylkill River
Christina River
Chesapeake Delaware Canal
Smyrna River

Figure 1 - Segmented Water Quality Model of the Delaware Estuary

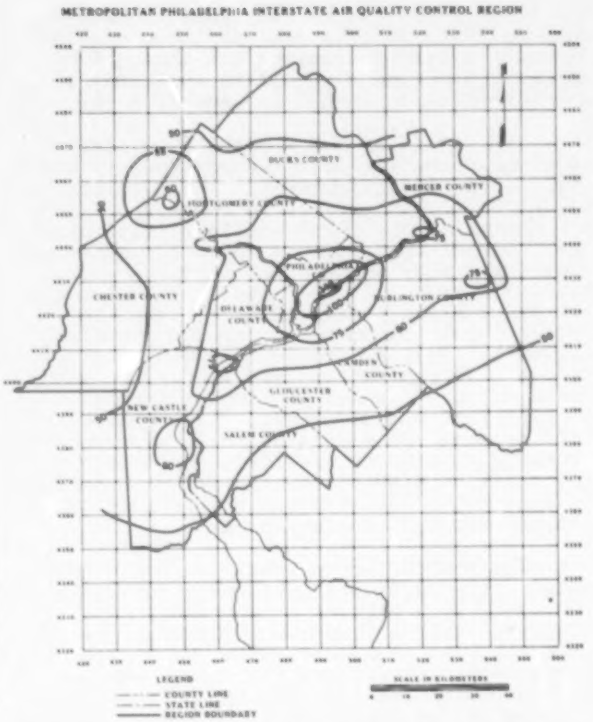
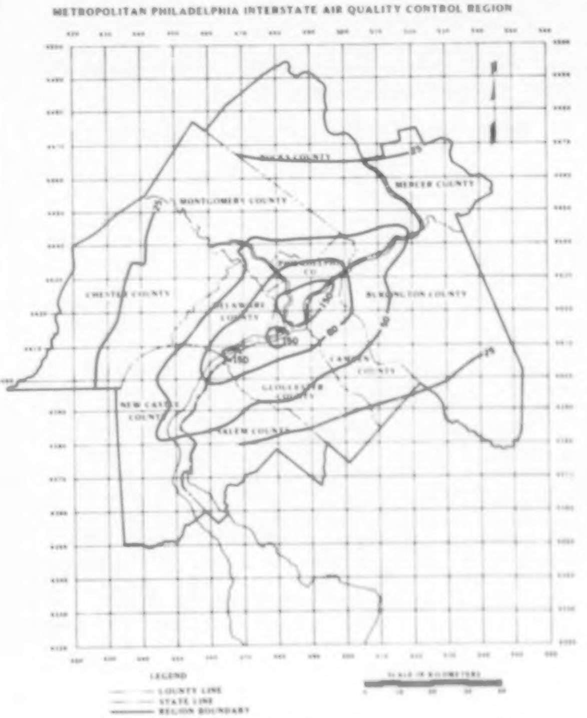

METROPOLITAN PHILADELPHIA INTERSTATE AIR QUALITY CONTROL REGION
BUCKS COUNTY
MONTGOMERY COUNTY
MERCER COUNTY
PHILADELPHIA
CHESTER COUNTY
DELAWARE COUNTY
BURLINGTON COUNTY
CAMDEN COUNTY
GLOUCESTER COUNTY
NEW CASTLE COUNTY
SALEM COUNTY
LEGEND
COUNTY LINE
STATE LINE
REGION BOUNDARY
SCALE IN KILOMETERS

Figure 2 - 1968 Annual Average Particulate Concentration (ug/m3)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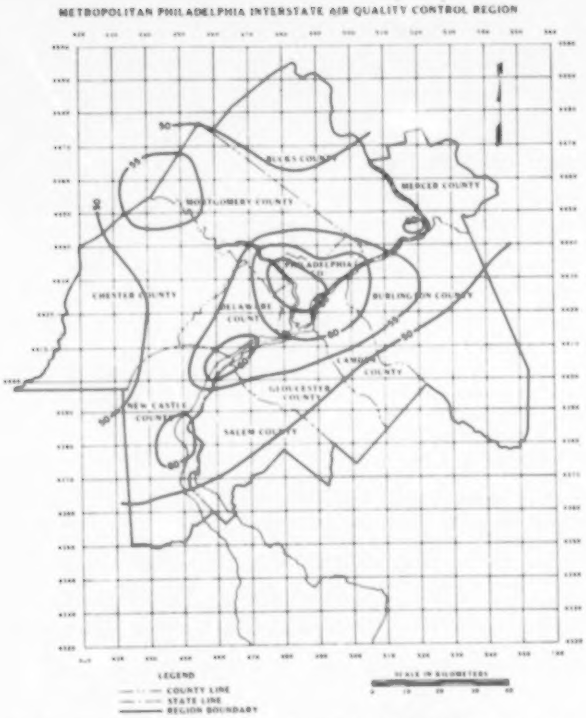
SCALE IN KILOMETERS

Figure 3 - 1968 Annual Average SO_2 Concentration (ug/m3)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NEW CASTLE COUNTY
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COUNTY LINE
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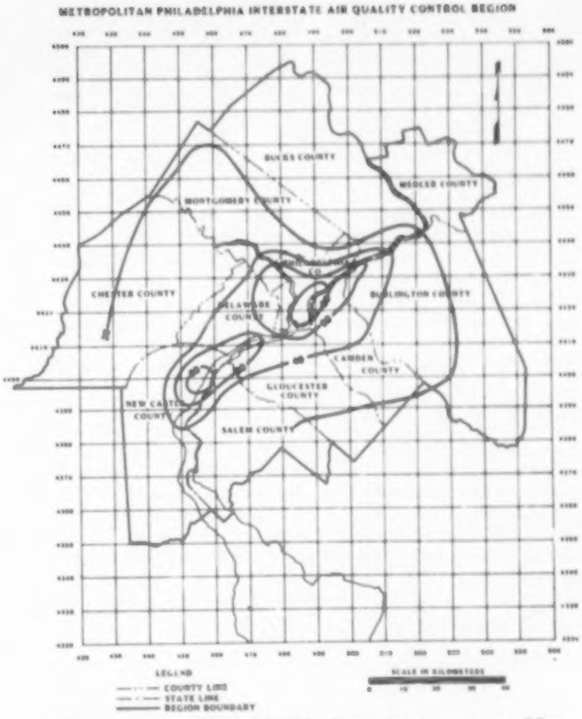
REGION BOUNDARY
SCALE IN KILOMETERS

Figure 4 - Resultant Annual Average Particulate Concentration (ug/m3)


METROPOLITAN PHILADELPHIA INTERSTATE AIR QUALITY CONTROL REGION
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SCALE IN KILOMETERS

Figure 5 - Resultant Annual Average SO_2 Concentration (ug/m3)

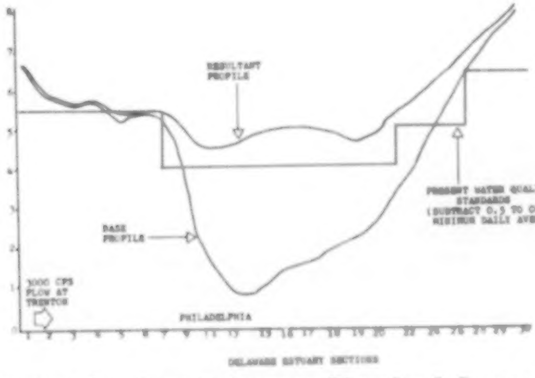

Figure 6 - Summer Average Dissolved Oxygen Profiles by Estuary Model Section (mg/l)

TOWARD A DYNAMIC ECONOMIC MODEL FOR REGULATING FLUOROCARBON EMISSIONS

Ralph d'Arge, Larry Eubanks, Joseph Barrington
Department of Economics
University of Wyoming
Laramie, Wyoming 82071

Abstract

A sequence of benefit-cost models is examined to determine economically feasible and optimal regulatory strategies for the production of chlorofluorocarbons by the United States. Estimates of environmental costs and market losses (consumer surplus) are developed to estimate at the margin where these costs balance each other. The implications of a dynamic regulatory model are briefly outlined.

Introduction

During the past decade, there has been a growing recognition that economic decisions might yield major impacts on global commons property resources, including the oceans, atmosphere, and even the electro-magnetic spectrum. Most recently, concern has been expressed as to the impact of chlorofluorocarbons on the ozone concentration in the stratosphere[1] and on the impact of these same compounds on world climate. According to the IMOS report,

> "Although the theory of possible ozone reduction (in the stratosphere) by fluorocarbons 11 and 12 (F-11 and F-12) cannot be presently supported by direct atmospheric measurements, the matter has been carefully studied independently by many scientists. Thus far, the validity of the theory and the predicted amounts of ozone reduction have not been seriously challenged. More research is required and will be undertaken, but there seems to be legitimate cause for serious concern."[2]

An extremely simplified sketch of this concern might be as follows: chlorofluorocarbons after or during economic use escape and ultimately collect in the stratosphere, a distinct air layer 11-60 kilometers above the surface of the earth. In the stratosphere these chemicals interact with ozone and other chemical constituents, initiating a reduction in ozone and perhaps a change to plants and animals, including humans. The climatic changes are presumed to induce another set of adjustments to organic life. The major question is whether, on balance, these changes in organic life are beneficial or adverse to humans. This is also the central question addressed, from an economic perspective, by the researchers authoring this report. Secondarily, a set of policy alternatives is examined as to the economic feasibility of alternative regulatory strategies. Typically such examinations are done with the aid of a cost-benefit analysis of the problem, and the results of such an analysis will be briefly summarized. In addition, possible steady state solutions to the question of optimal emissions is also examined. Finally, since the above two analyses do not indicate the optimal path to the optimal emission levels, and since there are differential emission rates for various uses of F-11 and F-12, a dynamic model of emissions is also outlined and discussed in an attempt to gain insight into the nature of the optimal path of emission reduction over time.

Cost-Benefit Analysis

The strategic point of the analysis was to examine market relationships for F-11 and F-12 and consumer products utilizing them and also to attempt to partially estimate the societal costs and benefits involved in their production and ultimate emission into the atmosphere.

Fluorocarbons for the most part are not purchased directly by households but are utilized as inputs to produce consumer products or services. In consequence, the observed demand relationships for fluorocarbons do not directly relate to consumer valuation but rather indirectly through demand for products utilizing fluorocarbons. Under some specialized circumstances, final product demand and consumer surplus will be exactly representable by the derived demand and surplus for fluorocarbons, such that observed losses in "derived" surplus would be equivalent to loss in consumer surplus in final goods markets. Unfortunately, observed data on prices and quantities sold historically may not adequately reflect actual dependencies between final product demand and surplus and derived demand and surplus. In order to obtain reasonable,valid bounds on "consumer surplus," both derived surplus and consumer surplus losses had to be estimated.

Measures of "derived surplus" loss for restrictions in fluorocarbon production were developed for F-11 and F-12 along with measures of consumer surplus loss for the major final products using these fluorocarbons in their production. Other fluorocarbons were not examined in detail by the authors. Included in the list of final products were: refrigerators, aerosol deodorants, auto air conditioners, polyurethane foam mattresses, and mobile vehicle refrigeration systems. According to the IMOS report, these products accounted for about 90% of utilization of major fluorocarbons and more than 98% of F-11 and F-12 use in 1972.[3]

Table 1 summarizes the empirical development of derived and final product demand relationships. Due to the relationship between derived and final product demand, it was believed to be the case that we were estimating demand relationships which were part of a simultaneous system of equations, and as a result the regression procedure known as two-stage-least squares was utilized as opposed to ordinary least squares in order that consistent coefficient estimates could be obtained.[4] Table 2 presents the set of willingness to pay estimating equations which were derived from the estimated derived and final product demand relationships in Table 1.

In Table 3 are recorded estimates of the present value of derived surplus for F-11 and F-12 and consumer surplus for major consumer products using F-11 and/or F-12 in their production. Such estimates were derived using the equations in Table 2. As is readily apparent from the estimates, "derived surplus" estimates amount to about $3 billions, while consumer surplus for the major products using them amount to more than $84 billions. Of course, these estimates would tend to bound the actual value of consumer surplus. On one extreme, if no substitutes existed for producing the final product, then the appropriate measure of economic loss would be the sum of consumer surplus losses in the final markets impacted. Whereas, if there were such substitution possibilities it would appear appropriate to utilize the "derived surplus" estimates.

It has been hypothesized that F-11 and F-12 emissions will induce two global effects:

1) reduction in stratospheric ozone and increase in UV-B light at the earth's surface
2) a slight rise in surface temperature due to an increased transparency of the stratosphere resulting from ozone depletion.

Both of these global effects, if they occurred at a significant level, would have large scale ramifications on biological life and thereby on the U.S. and other nations' economies. It would seem to be impossible to empirically estimate the thousands of interrelated impacts of changes in surface microclimates. In the partial analysis which was undertaken, costs and benefits are estimated for some major sectors of the U.S. economy from ozone depletion or enhancement and for slight long increases in surface temperature. The U.S. sectors and/or components of them included:

1) Ozone depletion
    1.1 Non-melanoma skin cancer
    1.2 Materials weathering (polymeric materials)

2) Temperature change (induced by ozone depletion)
    2.1 Marine resources (13 economic species)
    2.2 Forest products
    2.3 Agricultural crops (corn and cotton production
    2.4 Urban resources (fossil fuel, electricity, housing, clothing and government expenditures).

Estimated environmental costs and benefits by category for 1973 levels of emissions continuing into perpetuity are recorded in Table 4.

The major question is whether, given the evidence, F-11 and F-12 should be regulated as to production and/or emissions and to what degree. It is clear from a simple comparison of Tables 3 and 4 that the present value of net benefits of a complete ban on fluorocarbons production is positive if "derived surplus" is used as a measure of social cost and negative if the sum of "consumer surpluses" is used as the relevant measure. These conclusions are summarized in Table 5.

From Table 5 several general conclusions can be inferentially drawn. These are:

1) A complete ban on F-11 and F-12 may or may not be economically feasible depending on the availability of substitutes. The benefit-cost ratio for a complete ban may range from 0.2 to more than 6.0.

2) A partial ban on F-11 and F-12 use in products other than as a refrigerant appears to be economically feasible, although a major end use, hair sprays,^{5} has not been included in the benefit-cost comparisons.

3) If the hypothesis that fluorocarbon emissions affect temperature through altering the amount of ozone and thereby light reduction is not true, then the economic feasibility of a total ban is questionable.

Steady State Analysis

The benefit-cost analysis in the preceeding section indicated the circumstances under which a complete or partial ban on F-11 and F-12 might be economically feasible. This analysis is supplemented in this section by an examination of the optimum "steady state" percentage reduction in the production of fluorocarbons.

The optimum "steady state" percentage reduction in the production of fluorocarbons can be defined as occurring when total costs, including surplus losses and environmental costs, is at a minimum. This optimization problem can be written as:

$$\min. \quad S(Q) + EC(Q) \qquad (1)$$

where S(Q) denotes consumer surplus losses which are a function of the percentage of 1973 production of F-11 and F-12, Q, and EC(Q) denotes the environmental costs as a function of Q also. The necessary and sufficient conditions for an optimum are given by:

$$S'(Q) + EC'(Q) = 0 \quad \text{or} \quad S'(Q) = - EC'(W) \qquad (2)$$
$$S''(Q) + EC''(Q) \geq 0$$

where (') and (") denote first and second derivatives respectively.

For the purposes of this optimization, both S(Q) and EC(Q) have been estimated. The best estimator of S(Q) appears to be by a parabolic function. Three possible S(Q)'s were estimated for various measures of consumer surplus. The estimated S(Q) functions are presented in Table 6. The first function uses derived surplus as the measure of surplus loss, the second function uses consumer surplus, and the final function uses consumer surplus utilizing the assumption that substitutes for refrigerants exist after ten years and substitutes for propellants and foams are available immediately.

It was observed that the relationship between environmental cost by category in present value terms and U.S. production of F-11 and F-12 approximated a straight line over the range of interest. Thus, the estimation of the chain of events of production to emissions, emissions to changes in UV light and temperature, changes in UV light on materials life and skin cancer, and temperature on urban plus natural resources, and finally conversion of these physical-biological impacts into discounted (at a constant rate) economic costs can apparently be approximated by a linear relationship. The approximate linear relationship occurred for both temperature and UV related environmental costs. These estimated linear relationships are presented in Table 7. In order for the environmental cost functions to be comparable with the surplus loss functions at given "steady state" long run reductions in U.S. production, those occurring in the distant future had to be discounted back to the present then annualized. Thus the estimated EC(Q) presented in Table 7 represents annualized environmental costs for the various discount rates (3%, 5%, and 8%).

The results of the minimization problem represented by (1) are summarized in Table 8. It is important to note that Q is only defined over the interval [0,100] since it represents percentage of 1973 production of F-11 and F-12. As such, any solution presented in Table 8 for which either $Q \leq 0$ or $Q \geq 100$ represents a "corner solution" and corresponds to either a 100% optimal reduction in production or no reduction in production, respectively. Since Q denotes percentage of 1973 production of fluorocarbons, the optimal reduction in fluorocarbons is given by 100-Q. The important conclusion of this "steady state" optimization analysis is that the determination of the optimum is dependent both on the possibility of substitutes for fluorocarbons in final products as well as whether the environmental impacts are likely to be associated with UV increase or also with climatic change.

The possible policy alternative would be to assume that discretionary power existed which would allow regulators of fluorocarbons to specify which final products would be allowed to utilize F-11 and F-12 in their production. For purposes of making such policy decisions, one reasonable strategy might be to eliminate use of F-11 and F-12 first in those products which provide the smallest loss in consumer surplus per pound of fluorocarbons used in the production of the product. If crude estimates are made of average consumer surplus generated in dollars per pound of fluorocarbon by type of consumer product, one obtains a range of from 18¢ per pound for deodorants to $272 per pound for refrigerators. Figure 1 illustrates the optimal "steady state" under this assumption of discretionary power where the loss in consumer surplus function is derived by assuming complete elimination of final products utilizing fluorocarbons where the products are eliminated from smallest value of consumer surplus per pound of fluorocarbon to greatest value. In this case, a rather narrow optimum range of from 42 to 48% reduction in F-11 and F-12 is estimated as optimal. The products that could not be allowed to use F-11 and F-12 are: deodorants using propellants; perhaps hair spray; foam mattresses, and perhaps some type of refrigeration systems. It is to be noted that unlike the previous cases, the optimum strategy is highly insensitive to the discount rate applied to environmental costs.

A Prelude to Dynamic Analysis

The analysis of the preceeding section has indicated possible optimal "steady state" reductions in the production of F-11 and F-12, but such an analysis does not indicate the optimum path through time for regulation, i.e., it might pay to slowly approach the steady state optimum and only achieve it in two or three decades. The importance of this possibility is perhaps suggested by the observation that there are differential emission rates for each of the possible categories of final product uses of fluorocarbons, and also by the fact that at current emission rates an appreciable (2-4%) ozone depletion may not occur for 10 to 20 years and biological impacts 10 to 30 years after that. In addition, time lags in approaching the "steady state" would permit the development of adequate substitutes for some or all final products now dependent on F-11 and F-12. The dynamic model which is developed below will perhaps aid in an analysis attempting to discover optimal time paths toward the optimal steady state.

Development of the model best begins with a discussion of differential emission rates. There are, as was noted earlier, three major categories of fluorocarbon use: propellants, foaming agents, and refrigerants. Each of these uses causes emission of fluorocarbons into the atmosphere, but the rate of release is different in each case. Foaming agents release their emissions immediately upon use, while the assumption which is usually made with regard to propellants is that their emissions are released within six months of their production.[6] On the other hand, refrigerant uses release emissions at a much slower rate that varies from about two percent to 30% annually depending upon the type of refrigerant use.[7] Thus the dynamic aspect of the fluorocarbon emission problem which is of particular interest is the rate at which the emissions occur for the various product uses of fluorocarbons. If one denotes emissions by product Z_p, Z_f and Z_r for propellants, foams, and refrigerants respectively, structural equations for a model might be of the following form:

$$Z_f(t) = \beta_f Q_{ft} \tag{4}$$

$$Z_p(t+.5) = \beta_p Q_{pt} \tag{5}$$

$$Z_r(t+6) = \beta_r Q_{rt} \tag{6}$$

where the Q's would represent quantity of fluorocarbons used as foams, propellants, and refrigerants, and the β's give the emissions per unit of fluorocarbons in each use. $Z_r(5+6)$ was calculated as a weighted average of emission rates for refrigerants, using the assumption that all emissions are released at the end of the economic lifetime of the refrigeration final product in question; and the economic lifetime was assumed complete after 70% of the refrigerant had been emitted at given emission rates for the type of refrigeration final product being considered. For example, after a refrigerator had emitted 70% of its original charge it was assumed that the refrigerator was "scrapped" and as a result all remaining refrigerant was assumed emitted. This is an extremely simplified approach which does not include a more realistic representation of the depreciation process of the refrigerator nor its consequent source of emissions when it is no longer useful as a refrigerator. Total emissions of F-11 and F-12 can then be represented by:

$$Z_t = \alpha Q_t + Z_p(t+.5) + Z_f(t) + Z_r(t+6) \tag{7}$$

where αQ_t represents the quantity of fluorocarbons lost to the environment during production, transport, and storage.

Estimated values for the parameters in the above equations have been derived from the IMOS report and imply the following relationships:[8]

$$Z_f(t) = Q_{ft} \tag{8}$$

$$Z_p(t+.5) = .94 Q_{ft} \tag{9}$$

$$Z_r(t+6) = Q_{rt} \tag{10}$$

A representation for the production relationships between the total quantity of F-11 and F-12 and the quantities used as foams, propellants and refrigerants needs to be derived. A very simple relationship of this form would be:

$$Q_t = \gamma_p Q_{pt} + \gamma_f Q_{ft} + \gamma_r Q_{rt} \tag{11}$$

Such a relationship essentially represents a fixed coefficient production function which would not adequately reflect actual production decisions that would vary according to the relative profitability of applying fluorocarbons in the production of foams, propellants, and refrigerants. The following relationship was estimated using 1973 production data:[9]

$$Q_t = .65 Q_{pt} + .10 Q_{ft} + .25 Q_{rt} \tag{12}$$

Utilizing (8), (9), (10), and (12), a simple "mass balance" relationship is derivable:

$$Z(t) = .711 Q(t) + .25 Q(t-6) + .039 Q(t-1) \tag{13}$$

assuming the remainder of propellants escape into the stratosphere in the following year.

The next aspect, and perhaps the most difficult to deal with adequately, is describing the relationship between the production and use of fluorocarbons and environmental costs. Earlier in the paper it was indicated that the sort of causal chain involved is from production to emissions of fluorocarbons, from emissions to ozone depletion, from ozone depletion to increases in UV light and changes in climate, and from these changes to environmental cost impacts. However, this simple delineation of a causal chain has abstracted from the time element involved. For example, the impact of an increase in UV light on the incidence of skin cancer does not occur immediately with the change in UV light but rather may reach the new steady state incidence rate after approximately 80 years.[10]

The problem is one of relating environmental costs to ozone depletion because of its consequent impact on UV light and climate. Ideally, it would be desirable to estimate the following sets of relationships:

$$EC_t^1(O_{3_{t-z_1}}) \text{ and } EC_t^2(O_{3_{t-z_2}}) \qquad (14)$$

$$O_3(t) = O_3(t-1) + f(z_t) \qquad (15)$$

where O_3 denotes ozone concentrations in the stratosphere, EC^1 and EC^2 denote environmental costs associated with UV changes and climatic changes respectively, $f(z_t)$ denotes the functional relationship between ozone depletion and emissions of fluorocarbons, and $t-z_1$ and $t-z_2$ represent the appropriate time profiles for UV induced and climatic induced environmental costs. Unfortunately, such complete relationships have not been adequately estimated. The problem arises because estimates of ozone depletion resulting from F-11 and F-12 production presume "steady state" production levels into the indefinite future.

As a first approximation to the problem, environmental costs can be specified as a function of emissions. Recalling the discussion of "steady state" optimum in the previous section, it was observed that the relationship between production and annualized environmental costs was very nearly linear. It seems reasonable to assume that the relationship between environmental costs and emissions would also be approximately linear.

Net economic benefits from fluorocarbon production can be estimated as consumer surplus. The objective functional for this model could then be represented as the maximization of net benefits which is the difference between consumer surplus and environmental costs:

$$\sum_{i-1} B(Q_t)\eta^t - \sum_{i=1} EC(Z_t)\eta^t \qquad (16)$$

where η^t is a discount factor and the planning interval one to γ is given.

With these assumptions and solving this simple model utilizing the previously described relationships, two results are obtained regardless of the discount rate employed. First, if "derived surplus" measures of consumer surplus are used, it is optimal to immediately move to the optimum steady state. Second, if the sum of final product consumer surpluses is utilized (with the consequent assumption of no future substitutions), then it will never pay to alter 1973 U.S. production levels. Finally, if reductions in emissions can be achieved through improved recycling and reduced losses for refrigerants, then (with this model) production of U.S. F-11 and F-12 should be reduced through time at a rate which is directly related to the rate of reduced emissions from this source.

An estimate of the environmental loss in present value to the United States of a one year delay (from 1977 to 1978) in achieving a reduction of 90% in production is \$826 millions (at 5%). Alternatively, a one year delay would yield a gain of about \$89 millions if measured by derived surplus or \$2,471 millions if measured by final goods markets. These results further confirm the conclusions above. Continued research will hopefully identify, given alternative assumptions regarding the time rate of discovery of substitutes and recycling possibilities, a feasible dynamic path for regulation.

Footnotes

[1] H.J. Molina and F.S. Rowland, "Stratospheric Sink for Chlorofluoromethanes: Chlorine Atom-Catalysed Destruction of Ozone," Nature, Vol. 249 (June 28, 1974).

[2] Fluorocarbons and the Environment, Report of Federal Task Force on Inadvertent Modification of the Stratosphere (IMOS), Council on Environmental Quality and Federal Council for Science and Technology (June 1975).

[3] Fluorocarbons and the Environment (op. cit.) p. 88.

[4] For a discussion of simultaneous equation bias and estimation of simultaneous equations, see Jan Kmenta (1971), Elements of Econometrics, McMillan Co.: New York, or Henri Theil (1970) Principles of Econometrics, John Wiley and Sons, Inc.: New York.

[5] Hair sprays were not incorporated in the analysis due to an unavailability of adequate price data.

[6] Fluorocarbons and the Environment (op. cit) and Arthur D. Little, Preliminary Economic Impact Assessment of Possible Regulatory Action to Control Atmospheric Emissions of Selected Halocarbons, Draft Report, Vol. 1, EPA Contract No. 68-02-1349, Task 8 (July 1975)

[7] Arthur D. Little (ibid).

[8] Fluorocarbons and the Environment (op. cit), p. 91.

[9] Fluorocarbons and the Environment (op. cit.) p. 88.

[10] Pythagoras Cutchis, Estimates of Increase in Skin Cancer Incidence with Time Following a Decrease in Stratospheric Ozone, Paper P-1089, Department of Transportation, Climatic Impact Assessment Program, Washington, D.C.

Regression Equation[a,b,c]	$\bar{R}^2$ [d]	S.E.[e]	d.w.[f]
1) $Q'_{11} = 902.136 - 461.633(P_{11}) - 196.888(P_{12}) - 2048.090(P_{CO}) - .065(P_R)$ (138.992)** (521.080) (654.022) (1622.507)* (.016)** $- 10.167(P_{NR})^{**} - .004(P_Q)$ (2.700) (.655)	.9973	6.560	2.077^I
2) $Q_{12} = 1578.630 - 3167.013(P_{12}) - 918.681(P_{11}) - .160(P_N) - 2.334(P_Q)$ (230.634)*** (1070.166)** (1189.099) (.083) (1.380)	.9846	12.270	2.688^I
3) $Q_R = 2505.288 - 16.616(P_R) + 2.306(I)$ (316.330)* (6.957)** (.187)***	.9623	199.862	2.1850
4) $Q_D = -1898.632 - 2023.520(P_D) + 775.570(P_{SD}) + 1.360(I)$ (638.656)*** (988.948)* (323.633)** (.350)***	.9720	20.585	1.293^I
5) $Q_M = -3073.343 - 33.362(P_M) + 67388(P_{CH}) + 1.237(I)$ (1364.301)* (16.499)* (21.057)* (.253)***	.9793	120.081	1.5715^I
6) $Q_A = -4696.801 - 13.885(P_A) + 6.762(I)$ (3199.565)* (16.080) (.700)***	.9252	384.571	2.050^I
7) $Q_{MR} = -5811.897 - 17.625(P_{MR}) + 12.836(I)$ (103807.750) (18.673) (30.640)	.9994	3351.55	2.1521

Footnotes:

[a] Symbols: WTP = willingness to pay   Q = quantity   P = price   I = per capita disposable income

Where the subscripts have the following meanings:

11 = fluorocarbon 11	R = refrigerator
12 = fluorocarbon 12	D = aerosol deodorants
M = polyurethane foam mattresses	A = auto air conditioners
	MR= mobile vehicle refrigeration systems

[b] Values in parentheses are the estimated standard errors of the corresponding coefficient estimate.

[c] t-statistics for the estimated coefficients may be obtained by dividing the coefficient by its standard error and can be used to test the hypothesis that the value of the estimated coefficient is statistically different from zero. The following superscripts placed on the coefficient standard errors indicate that the coefficient is statistically different from zero at the

*90% level of confidence
**95% level of confidence
***99% level of confidence.

[d] $\bar{R}^2$ denotes corrected R^2.

[e] S.E. denotes the estimated standard error of the regression.

[f] d.w. denotes the Durbin-Watson statistic which tests for the presence of autocorrelation.

The symbol I attached to the statistic indicates the test for autocorrelation was inconclusive at the 95% level of confidence. For a complete description of the Durbin-Watson test, see Henri Theil (1971) Principles of Econometrics. John Wiley and Sons, Inc.: New York, pp. 199-201.

Table 1. Summary of Two-Stage Least Squares Regression Analysis

Willingness to Pay Equation	Annual Willingness to Pay 1973 Steady State (Millions of 1967 Dollars)
1) $WTP_{11} = -.001(Q_{11})^2 + [1.083-.430(P_{12})-4.399(P_{CO})-.001(P_R)-.002(P_{NR})$ $-.00001(P_Q)]\,Q_{11}$	146.380
2) $WTP_{12} = -.00015(Q_{12})^2 + [.498-.280(P_{11})-.00005(P_N)-.001(P_Q)]\,Q_{12}$	129.087
3) $WTP_R = -.036(Q_R)^2 + [171.370+.158(I)]\,Q_R$	2,700.380
4) $WTP_D = -.00025(Q_D)^2 + [-.839+.383(P_{SD})+.0007(I)]\,Q_D$	660.080
5) $WTP_M = -.016(Q_M)^2 + [-87.153+1.341(P_{CH})+.085(I)]\,Q_M$	73.777
6) $WTP_A = -.036(Q_A)^2 + [-678.483+.362(I)]\,Q_A$	1,086.720
7) $WTP_{MR} = -.039(Q_{MR})^2 + [-330.792+1.883(I)]\,Q_{MR}$	217.760

Footnotes:

Symbols: WTP = willingness to pay   Q = quantity   P = price   I = per capita disposable income

Where the subscripts have the following meanings:

11 = fluorocarbon 11	M = polyurethane foam mattresses
12 = fluorocarbon 12	A = auto air conditioners
R = refrigerator	MR= mobile vehicle refrigeration systems
D = aerosol deodorants	

Relevant 1973 Values:

Q_{11} = 329 million pounds Q_A = 6,462 units P_{CO} = $.031 per pound I = $2965
Q_{12} = 687 million points Q_{MR} = 68,997 units P_N = $700.31 per million cubic feet P_I = 66.0*
Q_D = 439,600,000 units
Q_R = 6,960,000* units P_{11} = $.160 per pound* P_{FE} = $3.40 per 1000 gallons (UPP) P_{CH} = 38.00*
Q_M = 1,722,000* units P_{12} = $.227 per pound* P_Q = 110.0* P_{SD} = 95.20

*These values are estimates because we were unable to obtain actual 1973 values.

Sources:

Bureau of the Census. Current Industrial Reports: Air Conditioning and Refrigeration Equipment (including warm air furnaces), Series MA-35M; Mattresses and Bedsprings, Series M25E; Industrial Gases, Series M28C.

Soap, Cosmetics and Chemical Specialties

Consumer Price Index

U.S. Department of Commerce. Survey of Current Business (1974)

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U.S. International Trade Commission

Table 2. Willingness to Pay (WTP) Estimation Equations and Estimated Annual Willingness to Pay Assuming 1973 as Steady State Values

Present Value 1973, 5 Percent Discount Rate
In Millions of Dollars

Commodity Type	Estimated 1973 Expenditures by Commodity**	Consumer Surplus or Derived Surplus (present value)
F-11	40	2,201
F-12	96	740
Refrigerators	1,386	39,727
Polyurethane foam mattresses	39	1,007
Aerosol deodorants	729	1,174
Auto air conditioners	489	16,473***
Mobile vehicle refrigeration systems	97	3,349

*Area under the derived demand curve less equilibrium purchases in 1973.

**Expenditures are estimated from the demand relationships rather than actual data since actual price may deviate slightly from predicted price as given by the estimated demand relationship.

***See Chapter II for explanation of the size of this estimate.

Table 3. Estimates of Consumer Surplus and Derived Surplus* For Selected Products, United States, 1971 Dollars

Category of Impact	Cost or Benefit*
1. Ozone Depletion	
1.1 Non-melanoma skin cancer	52 -206
1.2 Materials weathering	569
1.3 Biomass productivity	
2. Temperature Change (ozone induced)	
2.1 Marine resources	-661***
2.2 Forest products	-11,060
2.3 Agricultural crops	
2.3.1 corn	269
2.3.2 cotton	-16
2.4 Urban resources	
2.4.1 fossil fuel use	-5,719
2.4.2 electricity use	45,617
2.4.3 housing & clothing expenditures	-11,377
2.4.4 public expenditures	-696
TOTAL	16,357

*Costs are expressed as a present value of all future costs and benefits resulting from the emission of F-11 and F-12 produced in the year 1973 and maintained at that level into perpetuity. A five percent rate of discount was utilized to convert to present values. Estimated costs applying three and eight percent discount rates are tabulated in Chapter VI of this report.

**Non-melanoma skin cancer costs are estimated at $325 per case and $1,292 per case. See Chapter IV and Appendix 6 for justification.

***Negative sign denotes benefit.

Table 4. Estimates of Environmental Costs by Category Due to Current Levels of F-11 and F-12 Emissions, United States, 1973 into Perpetuity (Million of 1971 dollars)

Measure of Cost and Benefit	Benefit* Estimates	Cost Estimate	Benefit-Cost Ratio
Derived Surplus	16,978-17,132	2,961	5.9
Final Product Consumer Surplus	16,978-17,132	81,720	.21
Derived Surplus (plus omission of temperature impacts)	621-775	2,942	.21-.26
Final Product Consumer Surplus (Refrigerators, mobile regrigeration systems and automobile air conditioning uses excluded)	9,598-9,596	2,181	6.6

*Measured by savings in environmental costs of 1973 level production of F-11 and F-12 in present value terms.

**Loss in consumer or derived surplus at 1973 use rates in present value terms.

***Approximation based on a 56% reduction in steady state emissions obtained from Fluorocarbons in the Environment (op. cit. Table VI-12

Table 5. Benefit-Cost Comparisons for a Ban On Production of Fluorocarbons 11 and 12 United States, 5 Percent Discount Rate (Millions of U.S. 1971 dollars)

A. Derived Surplus

$S(Q) = 147.006 - 2.935Q + .0146Q^2$

$S'(Q) = -2.935 + .029Q^2$

$S''(Q) = .029$

B. Consumer Surplus

$S(Q) = 4086.704 - 81.755Q + .409Q^2$

$S'(Q) = -81.755 - 818Q$

$S''(Q) = .818$

C. Consumer Surplus with Substitution Assumption[c]

$S(Q) = 3977.708 - 79.550Q + .398Q^2$

$S'(Q) = -79.55 + .796Q$

$S''(Q) = .796$

[a] Q ≡ percentage 1973 production of F-11 and F-12

S(Q) surplus loss function

[b] Q is defined only over the range [0,100]

[c] The assumption about substitution is that there are immediate substitutes for foams and propellants and substitutes for refrigerants after ten years.

Table 6. Estimated Surplus Loss Functions[ab]

Discount Rate	Intercept	Slope	r^2
Total Environmental Cost			
3%	184.94 (55.36)	15.87 (1.04)	.98
5%	96.08 (36.57)	7.61 (0.68)	.96
8%	23.23 (22.77)	1.96 (0.43)	.81
Skin Cancer and Materials Weathering Costs			
3%	6.29 (0.78)	0.46 (.015)	.99
5%	5.89 (0.46)	0.33 (.01)	.99
8%	3.88 (0.20)	0.16 (.01)	.99

*The estimated equation was $y = a + bx$ where y equaled annual costs commencing in 1973 in millions of 1971 U.S. dollars and x equaled the percentage of 1973 U.S. production of F-11 and F-12.

Table 7. Equations* Used to Approximate the Relationship Between Environmental Costs and U.S. Production Level of Fluorocarbons 11 and 12

I. Optimization Using Derived Surplus

		UV Related EC(Q)[d]	Total EC(Q)[e]
Discount	3%	Q = 100	Q = 0
Rate for	5%	Q = 100	Q = 0
EC(Q)	8%	Q = 100	Q = 49

II. Optimization Using Consumer Surplus

		UV Related EC(Q)[d]	Total EC(Q)[e]
Discount	3%	Q = 99	Q = 85
Rate for	5%	Q = 99	Q = 90
EC(Q)	8%	Q = 99	Q = 97

III. Optimization Using Consumer Surplus and Substitution Assumption

		UV Related EC(Q)[d]	Total EC(Q)[e]
Discount	3%	Q = 99	Q = 99
Rate for	5%	Q = 99	Q = 95
EC(Q)	8%	Q = 99	Q = 97

---

[a] Solutions are obtained by solving the necessary conditions $S'(Q) = -EC'(Q)$ for Q. Note that the sufficient conditions, $S''(Q) < -EC''(Q)$, hold in every case. Since EC(Q) is linear $EC''(Q) = 0$, and from Table 6 it can readily be seen that $S''(Q) < 0$ in every case.

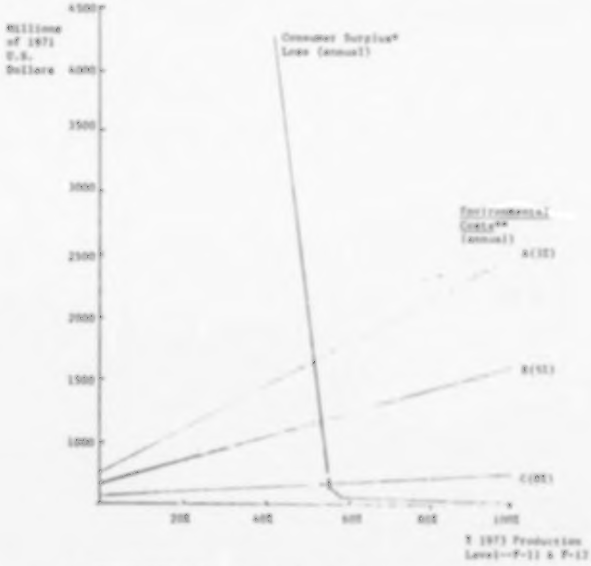
[b] Q ≡ percentage of 1973 F-11 and F-12 production
EC(Q) ≡ environmental costs

[c] $Q \leq 0$ or $Q \geq 100$ represents a "corner solution" and corresponds to $Q = 0$ and $Q = 100$ respectively.

[d] UV related environmental costs represent skin cancer and materials weathering costs, and the appropriate relationships can be found in Table 7.

[e] Total environmental costs included both UV and climate related costs. For appropriate relationships see Table 7.

Table 8. Solutions for Optimum "Steady State" Reduction in F-11 and F-12 Production[abc]



*Consumer surplus loss where products are removed according to rank order of loss per pound of fluorocarbons.

**Total environmental costs including both UV and temperature effects. Cases A, B, and C refer to application of 3, 5, and 8 percent social rates of discount, respectively.

Figure 1. Annual Consumer Surplus Losses With Product Ranking and Environmental Costs, United States, 1973

ENVIRONMENTAL, FISCAL AND SOCIO-ECONOMIC IMPACT OF LAND USE POLICIES: TOWARD AN INTERACTIVE ANALYSIS

J. Kühner, M. Shapiro, R.J. deLucia
Meta Systems Inc
Cambridge, Massachusetts

W.C. Lienesch
Water Planning Division
Environmental Protection Agency
Washington, D.C.

Summary

Effective implementation of recent environmental quality legislation requires planning tools which give quantitative estimates of the various impacts of land use and environmental controls. A literature review revealed that no adequate comprehensive tools are available. Three models have been developed by Meta Systems Inc for EPA in a recent study. They evaluate: (1) impact of urban nonpoint sources on water quality; (2) sewer and treatment plant capacity; and (3) distribution of costs borne by different groups in response to new development and environmental controls.

Introduction

Federal, state, regional and local environmental and land use policies have impacts on the physical environment and on local governments' economic and fiscal conditions. The impacts have been recognized in a qualitative manner, but there are few appropriate tools to quantify them. If land use and emission controls are to be used effectively in implementing environmental policies, it is necessary to consider the dynamics of the local environment in which these controls are being imposed. The availability of interactive computer models would permit local and regional planners and decision makers to look at the interactions and impacts described above. Ideally, such models should enable planners to consider all receiving media (air, water, land) and take into account the processes which transfer residuals from one medium to another.

Meta Systems recently completed a project for EPA which emphasized urban land use/environmental quality relationships.[1] Figure 1 is a conceptual model of the interactions between land use and environmental quality. This model provided a general framework for analysing relationships and for organizing a review of literature on models and emissions (see deLucia, et al.[2]). However, the project concentrated on the development of three types of models: (1) models for assessing the environmental impact of urban stormwater runoff, (2) a model for evaluating the capacities of sewers and wastewater treatment plants; and (3) a cost distribution model for assessing the cost to be covered by different groups in response to new urban and suburban development. In addition, an extensive evaluation of air pollutant emissions was undertaken. In this paper we briefly describe the models developed during the course of the study and outline their potential applications.

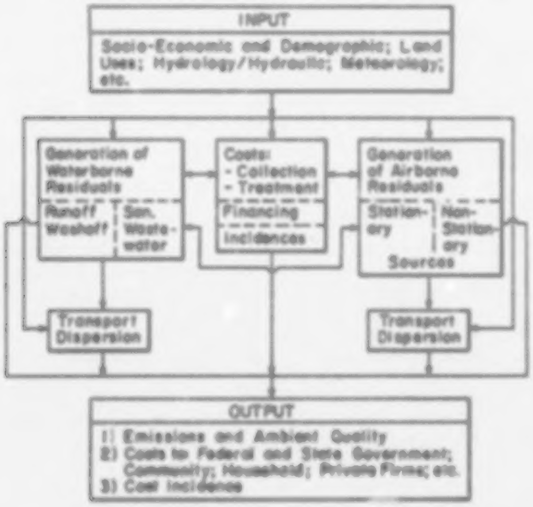

INPUT
Socio-Economic and Demographic; Land Uses; Hydrology/Hydraulic; Meteorology; etc.
Generation of Waterborne Residuals
Runoff Washoff
San. Waste-water
Costs:
- Collection
- Treatment
Financing
Incidences
Generation of Airborne Residuals
Station-ary
Non-Station-ary
Sources
Transport Dispersion
Transport Dispersion
OUTPUT
1) Emissions and Ambient Quality
2) Costs to Federal and State Government; Community; Household; Private Firms; etc.
3) Cost Incidence

Figure 1: Conceptual Model for Urban Land Use Environmental Quality Relationships

Descriptions of the Models

Urban Runoff and Washoff

Urban runoff produces about the same order of magnitude of pollutant as secondary effluent from separately treated sanitary sewage, with the exception that it is somewhat lower in total nitrogen and higher in sediment.[2] Thus maintenance and improvement of water quality requires methods for predicting the impact from runoff associated with urban land uses. We have combined a dynamic water quality model with a rainfall-runoff-model; the resulting program can be used for investigating the impact of land uses and urban land management (such as street sweeping) on the quantity and quality of stormwater runoff, and on the propagation of waves and pollutants in the receiving water body. After an intensive literature review[1,2], we decided to link together STORM[3] and the dynamic receiving water body model of SWMM[4], two publicly available computer models. STORM, a continuous model, is attractive because of its relative simplicity of use. The data required for the model are not very detailed and appear to be available in most areas. These data include land use categories, terrain description, pollutant loading, runoff coefficients, antecedent conditions, available storage and treatment, erosion potential and precipitation record. The major drawback of the model is its simplified approach to the runoff coefficient; it uses an adjusted rational formula containing a composite runoff coefficient. STORM is designed to compute urban as well as non-urban runoff and washoff. For every hour of runoff, hydrographs as well as pollutographs are generated. Pollutants included are suspended solids, settleable solids, BOD, N, PO_4, and coliforms (MPNs). STORM does not have any routing routines so that the application is limited to areas of less than approximately 10 square miles.

SWMM has two distinct phases (hydrodynamic and quality) which may be simulated together or separately. In the first phase, the equations of motion and continuity are applied to derive the hydrodynamics of the system for each time step, while in the second phase concentrations of conservative and non-conservative quality constituents are computed by using the first phase results and equations for conservation of mass. Information requirements are similar to those of the steady-state models.[5]

A considerable amount of time and effort has gone into restructuring STORM and SWMM to link the two programs and make them compatible. The major modifications completed are presented in Table 1.

Table 1

Changes in STORM (A) and SWMM (B)
for an Efficient Linkage

(A) -- $^{H}_{P}$ GPH* files have been created to pass results from STORM to SWMM
-- Rain interval is used instead of rain event for file generation
-- Erosion is calculated hourly
-- Erosion is accumulated over the rain interval
-- Eroded material can be added to suspended solids
-- Coliforms are included as sixth pollutant
-- Program calculates amount of dust and dirt accumulated at the beginning of rain interval, and amount left over after the rain event
-- Numerous bugs in the original program have been corrected (logic, core, program, files, default).

(B) -- $^{H}_{P}$ GPH files are accepted as sequential input
-- One or more of the six pollutants can be selected for individual runs
-- Quality phase can be run independently of hydrodynamic phase
-- Adjusting factors introduced for $^{H}_{P}$ GPHs.

---

* $^{H}_{P}$ GPH means hydrograph and pollutograph.

The linkage provides two points of interaction for the planner. First, he can choose specific rain intervals from the continuous simulation period of STORM. Then he can select those intervals from STORM's output of pollutographs and hydrographs, to be passed on to SWMM. This option significantly reduces the computing costs, but still allows for simulation of all the events if computation of a frequency distribution of conditions is desired. Water quality computations for specific pollutants can be done separately from the hydrodynamic computations by varying pollutograph inputs generated for each point discharge of runoff. This permits intensive testing of quality related parameters and thereby facilitates calibration of the quality model.[5]

The following types of output can be generated by STORM and SWMM: (1) hydrographs and pollutographs as total/year/sub-basin or as total/rain interval/sub-basin or as total/hour/sub-basin; (2) the amount of dust and dirt on impervious areas at the beginning and end of rain intervals; (3) total erosion for selected rainfall events and the amount finally reaching channels (stream) after application of a sediment delivery ratio; (4) stage of water level at each selected node of the river system for every rainfall event; (5) water level at every node of the river system for each day; (6) velocity and flow in every channel of the river system for each day; and (7) hourly concentration of selected pollutants at every selected node.

Capacity Evaluation Model

The capacity evaluation model enables planners to predict when and where new sanitary sewer and wastewater treatment plant capacity will be needed to accommodate projected development. This capability enables planning to begin on relief sewers before environmentally disruptive back-ups of main sewers occur. In addition, the information provided by the capacity evaluation model provides one of the elements needed to project the fiscal impact of development. It is not the purpose of the model to replace the detailed engineering services provided by public works departments and engineering consultants. Rather it serves to warn planners when additional detailed (and expensive) engineering studies are required and indicates where the most significant problems are likely to occur.

The evaluation model works from two types of input data. One set of data contains land use and planning information, including land use projections and wastewater generation characteristics. The data set is organized by cells, which are geographic sub-regions of the planning area. Cells may be specified from rectangular grids, census tracts, or other classifications for which planning data are available.

The second set of data characterizes the collection network and employs a classification scheme adopted from a previous Meta Systems study.[6] The collection system is divided into a series of arbitrary links. Each link is assigned an identification number, and characterized by link type and by the number of the next downstream link.[1] This characterization enables the program to "reconstruct" the sewer network and evaluate link flows in a straightforward fashion. The program logic makes it possible to characterize virtually any realistic collection network, and allows for the inclusion of force mains and relief sewers.

The major output of the capacity evaluation model is a tabulation of maximum flows for each link in the network. This information is presented for four time periods: a base year and 10, 25, and 50 years from the base year. The projected flows are compared with maximum design flows of the links and the percent utilization and overflows (if any) are indicated. An additional program option allows similar results to be computed and listed for treatment plants located in the system.

The model uses steady state hydraulics; the ability of upstream links to store back-up from an overloaded line is not taken into account. Thus actual overflows are likely to be less than those predicted. However, the model is intended only to signal possible problems. More detailed evaluations should be performed when overflows are indicated.

Cost and Fiscal Impact Model

Because of the multiplicity of financing arrangements and the importance of considering the temporal aspects of financing, it is often difficult for a planner to work through the financial aspects of new development, particularly where many alternative development patterns and financing arrangements must be considered. The fiscal impact model is designed to help planners trace how the environmental infrastructure costs incurred by new development are reflected in fiscal demands upon the community and in charges to the individual consumer.

The structure of the impact model is depicted in Figure 2. Input data includes three types of information:

1. Socio-economic data describing the size and growth of the residential, commercial, and industrial land uses served by the facility; and data on the property values associated with these uses.

2. Facility data specifying the type and size of facility. Currently the program handles eight types of facilities: septic tanks, sanitary sewer laterals, sanitary sewer house-connections, sanitary sewer mains and trunks, storm sewer laterals, stormwater detention basins, storm sewer mains, and sewage treatment plants.

3. Cost allocation data specifying the mechanisms (e.g., user charges) used to finance the facilities and the cost shares allocated to each mechanism.

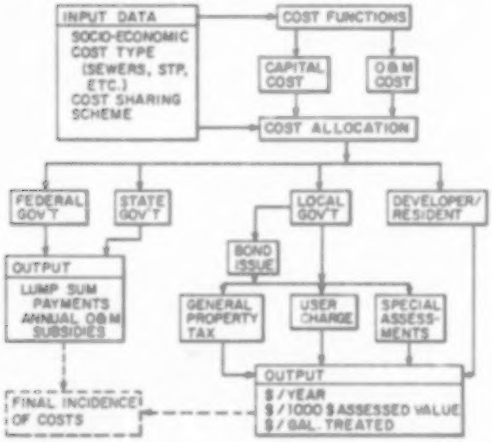


Figure 2: Logic of Cost and Fiscal Impact Model

Cost sub-models compute the capital and O&M costs for each facility type. These costs are then allocated to federal and state subsidies, local government, and developers or residents. The local government expenditures are further broken down into those financed through long term debt (mostly capital expenditures) and those financed through current revenues (mostly O&M expenditures). Finally the local expenditures are converted to assessments and user charges according to the input specification.

Output from the program includes several measures of fiscal impact: the time sequence of aggregate expenditures required by federal, state and local governments and the private sector, the time sequence of property taxes and user charges needed to finance the local costs, and measures of total costs borne by the consumer. The latter are computed by summing all charges (including private sector) paid by the consumer and converting to a constant base to yield an implied tax rate or user charge, i.e., the tax rate or user charge which would be required if all local and private expenditures were financed by a single mechanism.

A final desirable element of the model which has not yet been developed, is a sub-model for computing final cost incidence. This sub-model would provide the tax impacts of federal and state subsidies and the amount of commercial and industrial expenditures which are passed on to consumers inside and outside of the service area.

Examples of the Results

Results from the three models are not based on the same case study, but are drawn from different examples that best demonstrate the models' usefulness.

Stormwater Runoff Model

Results from the first model (Figure 3 and Table 2) are based on the analysis of the Mill River Basin, Hamden, Connecticut.

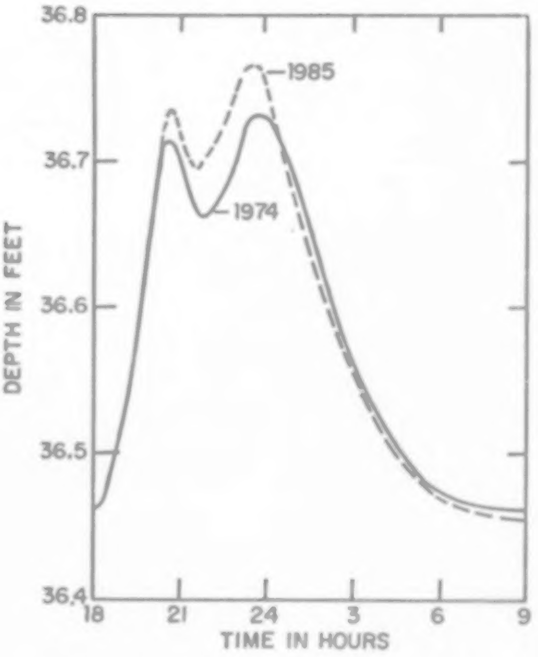


Figure 3: Stage Graph at Dam for 1974 and 1985

conditions: 3 hour rainfall interval with .51 inches of rain; low base flow

Table 2

Ratio of Coliforms from 1985 to 1974 Land Uses

conditions: 3 hour rainfall; .51 inches; low base flow

	Time (hour)	Junction Number 1 (dam)	3	6	8	11	12 (up-stream)
Rainfall	19:00	1	1	1.38	1.46	1.72	.51
	20:00	1.14	.95	1.41	2.18	.86	1
	21:00	1.03	1.28	1.60	4.06	.97	1
	22:00	1.4	1.38	1.89	1.9	1	1
	23:00	1.5	1.44	3.04	.81	.92	1
	24:00 (M)	1.55	1.47	2.44	1	.88	1
	2:00	1.57	1.67	1.27	.97	1	1
	6:00	1.43	1.68	2.24	1	1	1
	14:00	1.59	1.66	.19	1	1	1

The river has a drainage area (above the dam at Whitney Lake) of 37.7 square miles and is of triangular shape, about 13.5 miles long and about 5.5 miles wide at the upper end. During the 40-year period from 1918 to 1957 the average flow at the dam was 42 mgd. For the analysis we have divided the basin in 11 sub-basins. Mixed urban and non-urban land uses exist in the 11 sub-basins; 5,030 acres are considered developed in 1974 and 6,300 developed acres are projected for 1985.

In Figure 3 the peak stages at the dam are higher in 1985 than 1974, indicating the impact of increased development on runoff in the basin. In Table 2 the ratios of 1985 to 1974 coliform concentrations indicate that, at most junctions, additional development results in higher concentrations. However, due to the increased runoff, at some junctions and times coliform concentrations are actually reduced.

Capacity Evaluation Model

Table 3 illustrates the output from the capacity evaluation model for a hypothetical 12 link sewer network and associated treatment plant. The Table indicates that link 6 is likely to back-up under the proposed development scenario and that the efficiency of treatment will be somewhat reduced, as the capacity of the tertiary treatment facilities will be exceeded. As a next stage in the analysis, the planner could evaluate proposed relief sewers by adding appropriate links and re-running the model.

Table 3
Link Capacities and Flows for
Hypothetical Sewer Network

Full and/or Overcapacity Flows:

Link 6 flow exceeded the maximum capacity
by 12.7 percent (1.58 cfs)

Flow in Links (cfs)

Link ID	Max. Flow	Actual Flow	Percent Utilization	Cumulative Overflow
1	1.20	1.11	92.6	0.0
2	1.20	0.10	8.4	0.0
3	1.96	1.53	78.3	0.0
4	1.20	0.19	16.0	0.0
5	1.20	1.02	85.0	0.0
6	12.42	12.42	100.0	1.58
7	5.77	1.35	23.5	0.0
8	12.42	3.73	30.0	0.0
9	1.20	0.51	42.7	0.0
10	5.77	0.76	13.2	0.0
11	3.55	0.76	21.4	0.0
12	1.96	1.50	76.7	0.0

Total Flow Entering Treatment Plant (cfs) = 12.42

Treatment Plant Capacity

Stage	Maximum Capacity (cfs)	Percent Utilization
Primary	30.00	41.4
Secondary	20.00	62.1
Tertiary	10.00	124.2

Cost Impact Model

Table 4 represents one of the summary outputs available from the cost impact model. It lists aggregate expenditures for four infrastructure types required by a proposed new development of 890 dwelling units. The cost allocations employed are hypothetical and are not intended to correspond to existing practices. Costs are assigned to developers and local, state and federal governments. Within the local government category expenditures are further classified by revenue sources.

Table 4

Selected Costs of New Residential Development[*]

(590 townhouse units; 10 garden
apartments (30 du each))

Cost Type[**]	Developer	Local Gov't[***] A	Local Gov't[***] B	Local Gov't[***] C	State Gov't	U.S. Gov't
Sanitary Sewer Laterals						
Capital	303.7	0.0	60.7	182.2	60.7	0.0
O&M	0.0	0.0	1.5	0.0	0.4	0.0
Sanitary Sewer Interceptor						
Capital	278.0	222.4	0.0	0.0	5.6	0.0
O&M	0.0	0.0	0.2	0.6	0.2	0.0
Storm Sewer Laterals						
Capital	26.5	13.2	0.0	0.0	10.6	2.6
O&M	0.0	0.0	0.0	0.8	0.2	0.1
Storm Sewer Interceptor						
Capital	290.2	0.0	90.7	272.1	72.5	0.0
O&M	0.0	0.0	0.0	0.8	0.2	0.0

(*) All values are in thousand base year dollars. An entry of zero indicates the group or mechanism was not chosen for financing cost type.

(**) Capital costs are in thousand dollars per group or mechanism. O&M costs are in thousand dollars per year per group or mechanism.

(***) A = Special Assessment; B = User Charge; C = Property Tax.

Conclusion

The impact of federal, state, regional, and local environmental and land use policies on environmental quality is receiving increasing attention. Section 208 of the Federal Water Pollution Control Act Amendments of 1972, for example, requires the development and implementation of plans which include regulatory programs to control both point and nonpoint sources of pollution on an areawide basis.[7] Section 208 also mandates that land use controls be considered as measures to be included in the regulatory programs.

In addition, the 208 plans are to include a determination of the cost of the plan and a financial program to ensure that sufficient funds are available. It will be necessary, as part of the financial program, to determine the sources of funding, such as federal grants, user charges, property tax revenues, etc.

There is a need within the 208 and similar programs to determine more specifically the relationship between land use and environmental quality. Because many 208 agencies lack a quantitative understanding of the land use-water quality relationships for their particular areas, they may find it useful to follow the approach presented in this paper. Approaches such as this one do not provide definitive answers, but they do provide quantitative data that are more precise than the data which are generally available. This type of quantitative analysis will be necessary input to decisions which affect environmental quality.

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A TOTAL CONCEPT SYSTEM FOR MUNICIPAL WASTE DISPOSAL

Lester L. Nagel
Senior Project Engineer
Facilities Technology Division
Federal Facilities Office
U. S. Environmental Protection Agency - Region II
New York, New York

ABSTRACT

A review of the past and present means of waste disposal practices is given with individual evaluations of each.

The negative vs the positive mode of thinking with respect to waste disposal uses are discussed.

Based on the positive aspect element, two total concept systems are technically developed. Existing and proposed useful end product concepts are examined and evaluated.

Continuity is maintained by proceeding to examine the economic aspects of the respective systems proposed and how each relate, in its resultant cost estimate and to the ultimate financial impact on the community, to a system's capacity as well as on a per capita basis.

A summary of the success of the proposed systems to the basic criteria, as outlined in the "positive aspect" approach to the disposal problem, is given for each of the eight conditions initially cited.

BACKGROUND

The body of information presented in this paper is directed to those public officials and individuals concerned with the disposal of municipal wastes of all types and the design, development and economics of such a system.

The multi-disciplines involved require extensive knowledge in such divergent areas that individuals and/or responsible public agencies do not usually have compatible expertise such that the end result of such a comprehensive system can be evaluated.

It therefore seems appropriate for an individual, having extensive experience in such areas to propose this concept.

The author's approach is therefore directed to these technical individuals and officials involved in and responsible for a community's waste disposal problems.

GENERAL CONSIDERATIONS

The problems of todays living are both complicated and often dangerous to our existence. None however vex us more than those problems related to the disposal of the products of our daily waste. As we become more numerous, this waste problem increases in magnitude and at the same time becomes restrictive in the available means of its disposal.

According to our 1970 census statistics there were 916 communities in the United States having a population of over 25,000. Sixty-five (65) percent of them are concentrated in twelve states. At present there are more than 150 over 100,000 each; 26 of them exceed 500,000. These figures do not include any of their surrounding suburbs.

The need for a modern practical method of waste disposal has long been sought. Numerous papers and articles have been previously presented on the subject. (5,8,9,11,15,19,20,22,28,29,30,31,&32). In no instance however, has the solution encompassed the entire problem in terms of the domestic concept requirements.

This paper therefore, presents such means for a complete system for the disposal of all of a community's daily waste matter.

Additionally it focuses attention on the advantages of combining any existing sewage treatment and/or municipal incinerator facilities at a single location. Regardless of the type of wastewater treatment facilities available the flash evaporation of the wastewater effluent is not affected by the overall system's operations nor the number of treatment stages prior to the flash evaporator unit.

For simplification only, two wastewater systems are illustrated. In practical applications any wastewater treatment system is suitable to the proposed concepts presented.

BASIC PROBLEMS

The use of fire to dispose of wastes has long prevailed. We have designed, built and operated incinerators that are initially expensive, inefficient in operation, wasteful in the utilization of the energy produced, and are one of the major causes of air pollution in areas of concentrated population. (1)

We do not recognize the fact that what appears to be an acceptable solution in foreign concepts may not be the most practical answer to our domestic problems of waste disposal (5,8,15,19, 20 & 22).

Reviewing these waste disposal problems, their magnitude, the present methods used and our future requirements, we can summarize them as follows:

Each of us presently creates approximately 5 lbs. of waste refuse each day (6) (7). In addition we also create daily 0.2 lbs. of sewage matter. Both present a disposal problem. Means of disposal are limited and can be broadly classified as follows:

1. Landfill (all types)
2. Incineration
3. Energy &/or Materials Resource Recovery
4. Burning or dumping at sea
5. Sewage treatment
6. Septic systems

Numerous installations have attempted and are utilizing, to some extent, the heat value in the burning of refuse. (5,9,11,15,19,20 & 22). Its use, in most instances, is limited to the production of steam and/or electrical power for incinerator plant use. EPA has made demonstration grants for various other uses such as: refuse derived fuel, methane recovery etc.

Our utility systems' efficient production of electric power makes the use of this heat energy for such purposes expensive and wasteful except for metropolitan size installations. Efforts to utilize sewage waste matter have proved largely unsuccessful (13) and economically impractical.

Incinerator designs have changed little since their inception. Todays designs basically consist of a firebox with intricate grate designs. They are batch or continuous fed and, until the early 1960's were lacking sophisticated fire combustion controls. We have visited and been briefed by others on the success of foreign installations using low excess air firing concepts, apparently without any significant changes to our own methods on existing installations. (8,14) European grate designs (8,15,19) have proven far more effective than ours but are only lately incorporated into our incinerator units.

Our past control of stack emissions have been either non-existant or inadequate in design and/or effectiveness. (1) The installation of efficient APC equipment has been installed and evaluated only within the past few years. (21,23, 24)

Past and present trends seem more concerned with the architectural aspects of functional disguise and, after the initial operational fanfare, settle into their normal inefficient dirty routine operations. The present status of disposal procedures cannot continue to prevail; otherwise, the threat of disease could reach a level detrimental to the public's health. Barring further opposition to change some hope for a practical solution is possible.

The Total Concept Solution

Consider the problem without the chains of conventional ways and existing techniques. Let us review the asset possibilities of the two discarded products of our daily lives, refuse and sewage wastes. Both consist of organic and inorganic substances which are useless to us individually and are therefore collected and disposed of for us by central means.

At this point the most useful utilization of this matter must be considered. Economic evaluation presents the following considerations:

1. Steam and Elec. Power Generation
2. Composting
3. Fertilizer Production
4. Land Reclaimation
5. Pyrolysis
6. Water Distillation

The production of steam and/or electric power cannot be domestically justified economically except for large installations. Power can be purchased at a lower cost than produced in limited capacities.

Composting has been tried and also found not commercially competitive. (22) Fertilizer production has also failed both economically and because of odor problems. (16)

Land reclaimation is limited by available sites and creates gas and pestilence problems unless the fill consists of inert matter.

Pyrolysis has yet to achieve economic success.

The sixth consideration, that of water distillation, presents interesting possibilities. Few will dispute the creation of clean water, when processed by the utilization of waste products. Water distillation fuel costs range from 30 to 40 percent of the total process product costs. (2) (3) The development of a low cost distillation system utilizing. "Industrial Waste Heat" has been proposed (4) and other proposals also utilizing waste heat have previously been made (5). Prime consideration to the solution of such systems demand that it be functionally self-sufficient and at least partially self-supporting from an economic standpoint.

Two versions of the suggested "Total Concept System for Municipal Waste Disposal" are shown in Figures I and II.

Each fulfills the economic and engineering requirements as previously stated. The ultimate concept system, given in Figure II however will be shown to have several advantages over that of the system shown in Figure I and will also fulfill all of the engineering and economic requirements previously stated.

The common advantages of both systems are reasonably obvious.

Consolidation of the refuse and sewage services at the same geographical location results in lower overall initial plant site costs, personnel requirements and plant operating expenses. Incineration of all solids increases the potential heat energy available, helps stabilize the refuse heat value and produces a reasonably inert fill residue greatly reduced in volume and weight. The disposal problem is thereby diminished to a considerable extent. The use of the chemically treated sewage water to produce clean water for the various system functions shown plus the surplus available for outright sale, achieves the objective of the system's partial economic self-sufficiency. Auxiliary fuel costs are practically non-existant and the electric power purchased for either system costs less than when in-plant produced.

Additionally the system of Figure II will operate at a higher net economic efficiency by utilization of all of the resultant heat to produce clean water plus elimination of all boiler maintenance on the non-existant steam boiler.

Each system would utilize an incinerator unit of 300 tons per day capacity, however whereas the Figure I system unit would utilize a conventional incinerator-steam boiler arrangement, shown in Figure III, the Figure II system would consist of a three stage incinerator having as the final stage a kiln type rotating barrel (Volund) design direct gas discharge unit (19,22,26) as shown in Figure IV. Firing temperature of both systems would be in the order of 1800-2300F which insures elimination of stack odor possibilities.

The rotary kiln exit gases of the Figure II system would be precleaned by a cyclone collector and then directly utilized in a flash type water distillation unit (17). The ultimate production of clean water would be 2.4×10^6 GPD for the Figure I system and 2.7×10^6 GPD for the Figure II system. Each system would provide approximately 15,000 GPD for use in dissolving sewage treatment chemicals. Some small additional amount would be required for makeup for the Figure I system steam boiler. The balance in either system would be available for sale as boiler feed water or to supplement the community's water needs.

Both systems have the advantage of allowing for wide variations in the quantity of water produced, dependent upon the seasonal or even daily change in heat energy value of the incinerated matter.

The systems presented are representative of the size required for a community or group of communities having a total population of 100,000. Multiples of the system's units could be installed at a lower unit cost with a resultant increase in total investment return in the distilled water product produced for use and/or sale.

Table I presents the respective capital costs of equipment and plant investment for both systems. Annual costs and investment return value for each system are also included. All values are predicated on a single 300 ton per day unit (100,000 population) system. Based upon the data presented in Table I-A the net annual cost per ton of matter incinerated is $4.00 and $3.84 respectively.

These net costs are derived upon the basis of a total of 300 tons/day or 110,000 tons per year generated on a 365 day basis and being incinerated on a 345 day schedule of continuous operation each day at a 90/100% capacity level.

Refuse collection costs are not included, however they would normally be lower reflecting the savings in shorter hauling distances with the use of such a centralized system for small communities. Included are removal costs of the incinerated residue for use as adjacent landfill.

Credit for the distillate water produced has been calculated at the lowest prevailing rate of producing boiler feed water, $2 per 1000 gals. Present day costs of treated boiler feed water is in the order of $2 to $3 per 1000 gallons. No additional credit has been included in the Table I calculations over the lower cost figure.

For comparison purposes the relative costs for the same systems shown in Figures I and II are given in Table I-B where an activated Sludge Type of Sewage Process is utilized.

Three additional aspects of the system functions given in this paper should also be noted.

They are all economic in nature and are therefore of primary importance when the following conditions may prevail:

1. In metropolitan areas having an urban-suburban population of 1,000,000 or greater, the generation of electrical energy from the heat output of a 3,000 Ton per day incinerator-steam boiler unit (System Fig. I) becomes economically feasible.

In this modification the flash evaporator unit would be eliminated, however the treated sewage water would then become the condensing cooling water for the steam turbine.

2. Most communities, having a basic population of 25,000 or more, have installed, on a regional basis, sewage treatment facilities and in some instances a municipal incinerator.

Where either or both of these exist the initial investment for either of the basic systems proposed is substantially reduced.

3. A raw refuse waste classification system above and beyond the reclamation of the metals in the ash residue can be added to any of the proposed systems discussed.

The economic advantages however must be carefully examined on an individual installation basis before inclusion as part of the basic systems proposed.

CONCLUSION

As a result of the concepts and economic data as presented the following criteria has been established:

1. Current methods of refuse disposal only, indicates an annual per capita cost range of $3.50 to $8.00 (7, 24). With reference to Table I, the comparable net annual per capita costs, after proportionate value credit for the useful products produced is made, would be 63¢ and $2.16 (credit) respectively. Substitution of the activated sludge process plant would increase the per capita costs or reduce the credits by 20 percent (Table I-B).

2. Waste products can be disposed of at low cost and in a useful manner.

3. A system design in which the quantity of the useful product produced is not vital to the systems level of operation is established.

4. Disposal of the residue products are reduced to acceptable levels.

5. The resultant residue can be disposed of in a useful manner in small areas and without sanitary complications.

6. Annual expenses of administration, operation and maintenance are lower than existing methods in use.

7. The base unit system capacity and costs are favorable to suburban and rural areas. Transportation costs of the collected matter is therefore lower.

8. Plant expansion can be made without duplicating the expenses on initial planning, engineering or architectural services.

"A TOTAL CONCEPT SYSTEM FOR MUNICIPAL WASTE DISPOSAL," as presented in this paper, therefore meets the present and future needs and requirements of disposal, economic, size and effective pollution control for urban, suburban and many rural communities in the United States.

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SUMMARIES - TABLE I, I-A & I-B

PLANT CAPITAL COSTS
with
PRIMARY TREATMENT PLANT

	System I	System II
Equipment Investment	9,545,000	9,020,000
Plant Investment	1,570,000	1,535,000
Total Investment	$11,115,000	$10,555,000
Net Annual Costs (Credit)	63,000	($216,000)

NET ANNUAL COSTS CHARGEABLE TO EACH FUNCTION

		Unit Costs	
Function	Percent	System I	System II
Incineration/Ton	25	$4.00	$3.84
Distillation/M.gal	35	74.4¢	63.5¢
Sewage Treatment/10^6 gal	40	19.3¢	18.5¢

PLANT CAPITAL COSTS
with
ACTIVATED SLUDGE PLANT

Equipment Investment	11,715,000	11,220,000
Plant Investment	1,670,000	1,635,000
Total Investment	$13,385,000	$12,855,000

TABLE I
PLANT CAPITAL COSTS
EQUIPMENT INVESTMENT (INSTALLED)
PRIMARY TREATMENT PLANT TYPE

Item	Figure I	Figure II
1 Incinerator & Boiler (300 TPD) (incl. Fans)	1,700,000	-----
1A Incinerator (only) (300 TPD) (incl. Fans)	----	850,000
2 Mechanical collector	80,000	80,000
3 Figure I Distillation Plant (2.4 x 10^6 GPD)	3,000,000	-----
3A Figure II Distillation Plant (2.7 x 10^6 GPD)	----	3,400,000
4 Sewage Process Plant (10 x 10^6 GPD)	3,500,000	3,500,000
5 APC Unit (ESP)	300,000	300,000
6 Heating & Air Conditioning System	70,000	70,000
7 Odor Unit (not required)	----	-----
8 System Coordination (10% of Equipment costs and Installation)	865,000	820,000
Total Equipment Investment	$9,545,000	$9,020,000

All figures have been rounded to nearest $1,000.

PLANT INVESTMENT

Item	Figure I	Figure II
Waste Land (100 acres @ $1000/acre)	100,000	100,000
Architectural & Engineering Fees (7% of T.E.I. & Bldg)	720,000	685,000
Office & Operations	750,000	750,000
Building for Items #1, 3 or 3A & 4		
Total Plant Investment	$1,570,000	$1,535,000
Grand Total	$11,115,000	$10,555,000

ANNUAL COSTS

	Figure I	Figure II
A Fixed Charges 8.024% (5% - 20 years)	892,000	847,000
B Electric Power		
(a) Sewage Plant - 300 KW		
(b) Distillation - 110 KW	90,000	90,000
(c) Incineration - 600 KW		
C Chemicals		
(a) Distillation Plant ($H_2 SO_4$ @ 2.50¢/lb.)	50,000	55,000
(b) Sewage Plant	20,000	22,000
D Operating Costs		
(a) Wages & Salaries		
(b) Maintenance & Parts		
(c) Administration		
(d) Insurance 6% of Total Equipment and Plant Investment	667,000	633,000
(e) Solid Disposal 37,000 tons @ $1.12/ton (incl. 25% Incombustables)	42,000	42,000
	$1,761,000	$1,689,000

ANNUAL INVESTMENT CREDIT

Item	Figure I	Figure II
A Processed Water @ $2/1000 gallons		
(a) 2.4×10^6 GPD $4,800/day - 345 days	1,656,000	------
(b) 2.7×10^6 GPD $5,400/day - 345 days	-----	1,863,000
B Recovered Metals @ 38¢/Ton Raw Refuse Processed (110,000 tons/yr)	42,000	42,000
Total Annual Credits	$1,698,000	$1,905,000
Net Annual Costs (Credits)	$63,000	($216,000)

Table I-A

The following items and/or percentages of items are directly chargeable to incineration use:

Item	Percent Chargeable	System Figure I	Figure II
1	100	1,700,000	------
1A	100	-----	850,000
2	100	80,000	80,000
5	100	300,000	300,000
6	50	35,000	35,000
8	25	216,000	205,000
Land	60	60,000	60,000
A&E Fees	25	180,000	171,000
Building	50	375,000	375,000
	Total	$2,946,000	$2,076,000
Capital Incinerator		9,820	6,920
Plant Costs/Ton Capacity			

The following items and/or percentages of items are directly chargeable to distillation uses:

Item	Percent Chargeable	Figure I	Figure II
3/3A	100	3,000,000	3,400,000
6	25	17,000	17,000
8	25	216,000	205,000
Land	20	20,000	20,000
A&E Fees	33	240,000	229,000
Building	25	188,000	188,000
		$3,681,000	$4,058,000
Capital Distillation			
Plant Costs/GPD			
Capacity (2.4×10^6		$1,534	-----
(2.7×10^6		-----	$1,503

The following items and/or percentages of items are directly chargeable to Sewage Treatment uses:

Item	Percent Chargeable	Figure I	Figure II
4	100	3,500,000	3,500,000
6	25	18,000	18,000
8	50	433,000	433,000
Land	20	20,000	20,000
A&E	42	300,000	285,000
Building	25	187,000	187,000
	Total	$4,458,000	$4,443,000
Capital Sewage Plant Costs/GPD Capacity 10×10^6		$0.4458	$0.4443

NET ANNUAL COSTS CHARGEABLE TO EACH FUNCTION
(Based on Proportionate Net Annual Costs)

Function	Processed Per Year	%	Costs - Dollars/Unit System I	System II
Incineration	110,000 Tons	25	$4,00/Ton	$3.84/Ton
Distillation		35		
Figure I	828×10^6		74.4¢/M gal	----
Figure II	931×10^6		----	63.5¢/M gal
Sewage Treatment	$3,650 \times 10^6$gal	40	19.3¢/M gal	18.5¢/M gal

TABLE I-B
ACTIVATED SLUDGE TYPE PLANT - CAPITAL COSTS
(a) Equipment Investment - Installed

Item	Equipment	Figure I	Figure II
1	Incinerator & Boiler 300 TPD-Including Fans	1,700,000	-------
1A	Incinerator only 300 TPD-Including Fans	-----	850,000
2	Mechanical Collector	80,000	80,000
3	Distillation Plant 2.4×10^6 GPD	3,000,000	-------
3A	Distillation Plant 2.7×10^6 GPD	-----	3,400,000
4	Sewage Plant 10×10^6 GPD	5,500,000	5,500,000
5	Precipitator	300,000	300,000
6	Heat & Cooling System	70,00	70,000
8	System Coordination 10% of Equipment & Installation Costs	1,065,000	1,020,000
	Total Equipment Investment	$11,715,000	$11,220,000

PLANT INVESTMENT

	Figure I	Figure II
Land - 100 Acres @ $1,000/Acre	100,000	100,000
A & E Fees - 7% of T.E.I. and Building	820,000	785,000
Building - Item 1, 3, & 4	750,000	750,000
Total Plant Investment	$1,670,000	$1,635,000
Grand Total	$13,385,000	$12,855,000

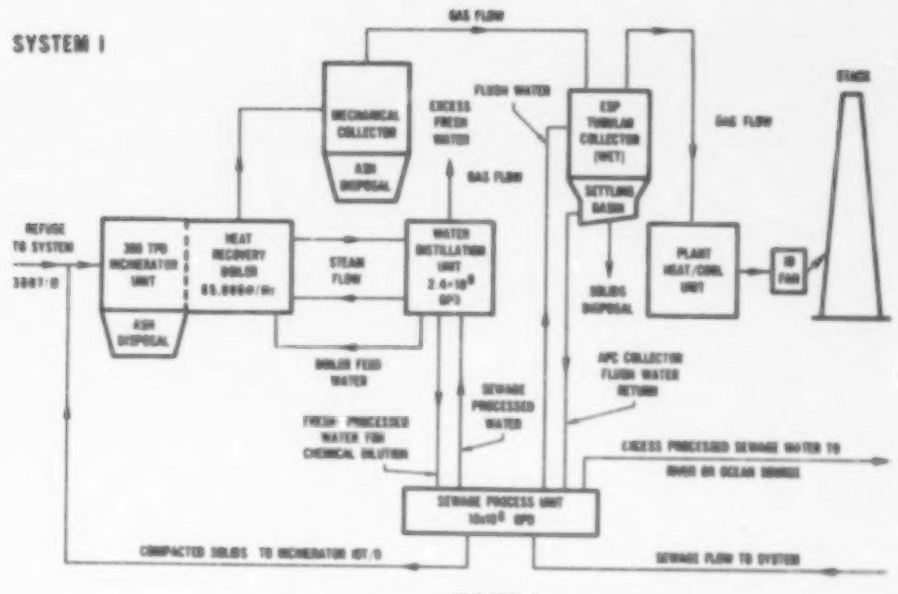
SYSTEM I
GAS FLOW
MECHANICAL COLLECTOR
ASH DISPOSAL
EXCESS FRESH WATER
GAS FLOW
FLUSH WATER
ESP TUBULAR COLLECTOR (WET)
SETTLING BASIN
GAS FLOW
STACK
REFUSE TO SYSTEM
300T/D
300 TPD INCINERATOR UNIT
ASH DISPOSAL
HEAT RECOVERY BOILER 85,000#/Hr
STEAM FLOW
WATER DISTILLATION UNIT 2.4×10⁶ GPD
SOLIDS DISPOSAL
PLANT HEAT/COOL UNIT
ID FAN
BOILER FEED WATER
SEWAGE PROCESSED WATER
APC COLLECTOR FLUSH WATER RETURN
FRESH PROCESSED WATER FOR CHEMICAL DILUTION
EXCESS PROCESSED SEWAGE WATER TO RIVER OR OCEAN SOURCE
SEWAGE PROCESS UNIT 10x10⁶ GPD
COMPACTED SOLIDS TO INCINERATOR 10T/D
SEWAGE FLOW TO SYSTEM

FIGURE I

TOTAL CONCEPT SYSTEM FOR MUNICIPAL WASTE DISPOSAL

(INCINERATOR-HEAT RECOVERY BOILER UTILIZATION)

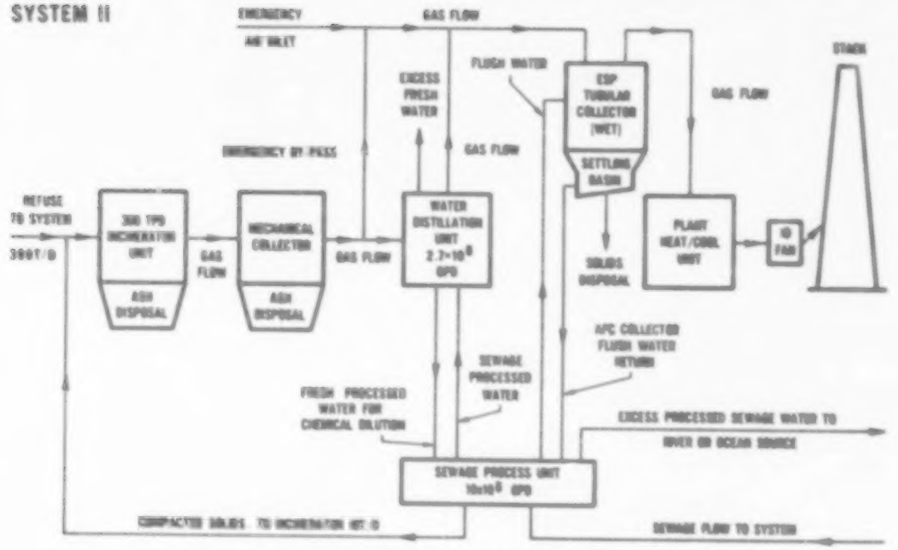
SYSTEM II
EMERGENCY AIR INLET
GAS FLOW
FLUSH WATER
ESP TUBULAR COLLECTOR (WET)
SETTLING BASIN
GAS FLOW
STACK
EXCESS FRESH WATER
GAS FLOW
EMERGENCY BY PASS
REFUSE TO SYSTEM
300T/D
300 TPD INCINERATOR UNIT
ASH DISPOSAL
GAS FLOW
MECHANICAL COLLECTOR
ASH DISPOSAL
GAS FLOW
WATER DISTILLATION UNIT 2.7×10⁶ GPD
SOLIDS DISPOSAL
PLANT HEAT/COOL UNIT
ID FAN
APC COLLECTOR FLUSH WATER RETURN
SEWAGE PROCESSED WATER
FRESH PROCESSED WATER FOR CHEMICAL DILUTION
EXCESS PROCESSED SEWAGE WATER TO RIVER OR OCEAN SOURCE
SEWAGE PROCESS UNIT 10x10⁶ GPD
COMPACTED SOLIDS TO INCINERATOR 10T/D
SEWAGE FLOW TO SYSTEM

FIGURE II

TOTAL CONCEPT SYSTEM FOR MUNICIPAL WASTE DISPOSAL

(ROTARY KILN WITH DIRECT GAS UTILIZATION)

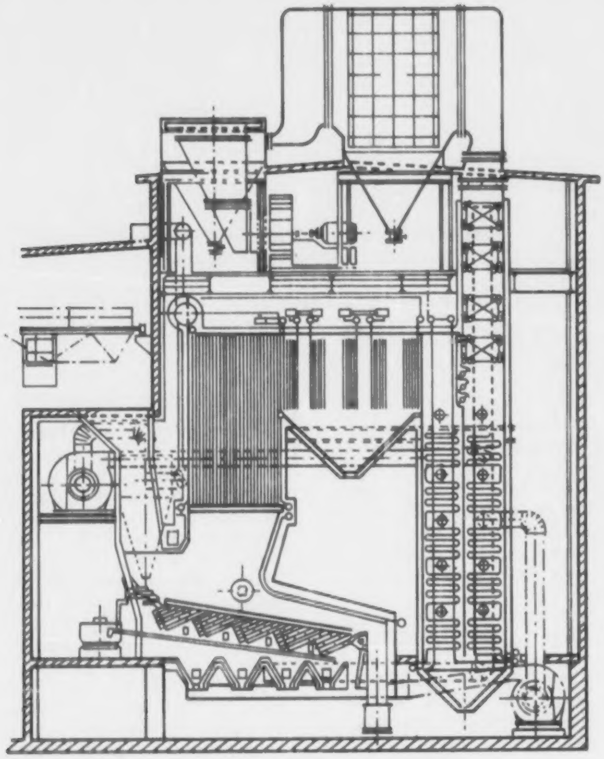

Figure 3. Boiler With Reciprocating Stroker

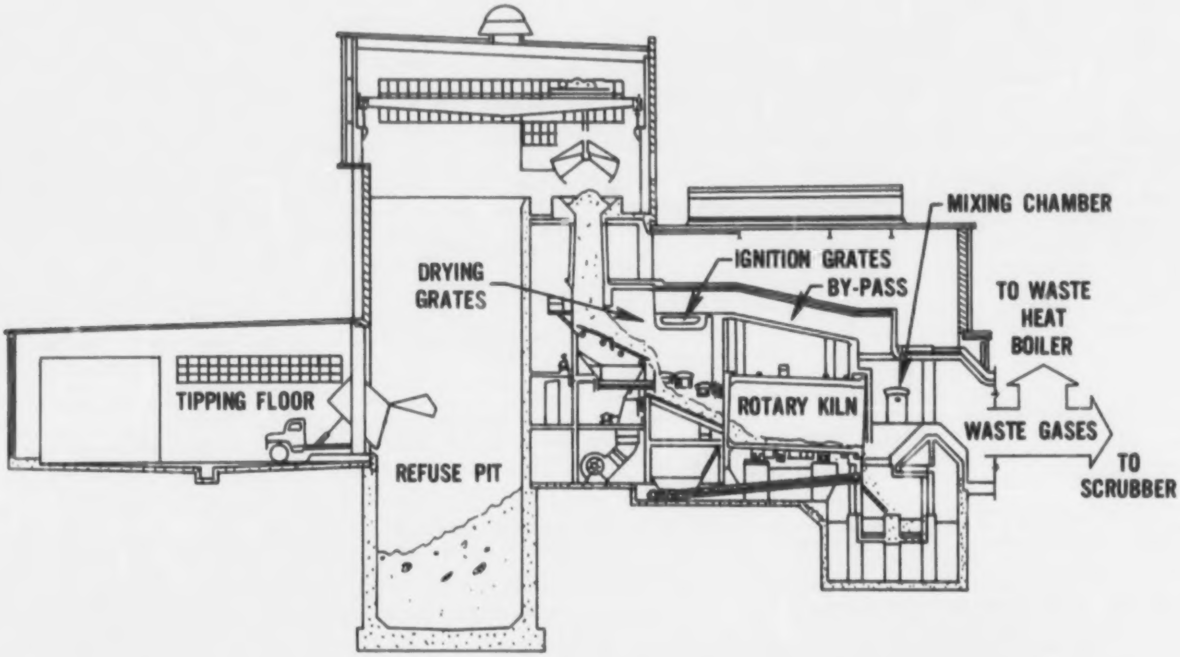
MIXING CHAMBER
IGNITION GRATES
DRYING GRATES
BY-PASS
TO WASTE HEAT BOILER
TIPPING FLOOR
ROTARY KILN
WASTE GASES
REFUSE PIT
TO SCRUBBER

Figure 4. Section Through Incinerator Unit

ECONOMIC FORECASTING FOR VIRGINIA'S WATER RESOURCE PROGRAMS

Charles P. Becker, Allender M. Griffin, Jr.,
Carol S. Lown

ABSTRACT

Water resource and water quality management planning depend, to a large degree, on forecasts of industrial activity and population projections. A flexible economic data base is especially important where planning follows varying formats of geographical and industrial detail. Records of employment and payroll are collected in the administration of Unemployment Insurance (U.I.) programs and are available from State Employment Agencies. These statistics have been collected over a long period of record (thrity-five years). Many years of record are available on punched-cards or magnetic tape and may be arrayed and manipulated by computer. This basic approach has been followed in Virginia. Historical U.I. payroll and employment records for the period 1956 through 1970 were procured on magnetic tape. This data was arrayed by major hydrologic area and by regional planning district. Projections of manufacturing activity were then generated by fitting several exponential equations to annual payroll data in two-digit Standard Industrial Classifications. These exponentials were then extrapolated to provide a range of industrial projections. Other parameters of manufacturing activity were then correlated to the payroll data to generate projections of indexes such as employment, value-added, and gross manufacturing output. U.I. payroll data is now being correlated to parameters in non-manufacturing categories. Projections for industries such as trade and services will link extrapolated payroll data with benchmark correlations of payroll and sales receipts.

(KEY TERMS: water resource planning; unemployment insurance (U.I.) statistics; value-added; exponential forecasting; population projections)

Economic data has played an important role in water resource planning and water quality management planning.[1] Parameters such as population, employment and value-added[2] in manufacturing have been correlated to water-use and waste generated. Water resource planning engineers and sanitary engineers are able to make predictive estimates of future water-use and waste levels by making correlations with various population and industrial projections. Water demand, expressed in millions of gallons per day (MGD) has been related to value-added in selected manufacturing categories. Water-use coefficients are also available for other heavy water-using industries such as mining. Domestic water demand can be predicted by applying per capita water-use factors to population forecasts. Parameters of water quality such as biological oxygen demand (BOD) and chemical oxygen demand (COD) have been correlated to economic indexes in major water-using industries. Relationships between per capita population and domestic waste generated have also been expressed quantitatively in terms of BOD and COD.

In order to produce valid economic forecasts for varying size planning units, the water resource economist must have a flexible and comprehensive data base. Traditional data sources, such as the Bureau of the Census — U. S. Department of Commerce, publish data[3] which provides a valuable overview to the water resource planner.

Often, however, more detailed, unpublished data is necessary where planning units follow a hydrologic format. Data by reporting establishment must be sorted and manipulated to produce a valid benchmark or forecast base for hydrologic planning areas of river basins. Of course, this same data may be sorted by county or city and further aggregated into economic planning regions.

The State Employment Security Agencies[4] have collected and stored an impressive record of payroll and employment data for administering Unemployment Insurance programs. This data has been collected in all of the states, in the territories of Puerto Rico and in the Virgin Islands. Unemployment Insurance (U.I.) laws vary somewhat from state to state in such areas as program detail and reporting coverage. Some states have, for example, full coverage in unemployment-insured industries. Other states have required U.I. reports from firms with four or more employees. Supplementary employment data may be obtained from he Federal Bureau of Old Age and Survivors Insurance (B.O.A.S.I.) of the Social Security Administration to bring coverage up to a universal or "100 percent" in these "partial coverage" states.

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[1] Between 1966 and 1972, the Virginia Division of Water Resources of the Department of Conservation and Economic Development was responsible for comprehensive water resource planning for the State of Virginia. On July 1, 1972, the Division of Water Resources was merged with the Virginia State Water Control Board. Since 1946, the Board has been responsible for water quality management in Virginia. The combined agency is now operating as the Virginia State Water Control Board.

[2] "Value-added of an industry consists of labor compensation, proprietors' income, profits, interest, depreciation, and indirect business taxes." (U. S. Department of Labor, B.L.S., 1970).

[3] In addition to an every-five year Census of Manufactures, the U. S. Department of Commerce. Bureau of the Census also conducts Annual Surveys of Manufacturing during interim years.

[4] The State Employment Security Agencies are affiliated with the Manpower Administration (formerly the Bureau of Employment Security of the U. S. Department of Labor.

The State of Virginia provides a good illustration where U.I. coverage was partial for years (required of firms with four or more employees) in unemployment insured industries. An amendment (effective January 1, 1972) to the Virginia U.I. law extended coverage to firms with one or more employees in unemployment insured industries. Certain types of employers are still excluded from U.I. coverage. Federal and local government, railroads, churches and state government (except non-teaching staffs of hospitals and institutions of higher learning) remain exempt from U.I. coverage.

All states, Puerto Rico and the Virgin Islands submit U.I. employment and payroll data to the Manpower Administration under the report designation Employment Security (E.S.) 202. The E.S. 202 report is forwarded in the form of a computer print-out. This record (E.S. 202) is assembled using individual establishment reports, i.e., the Employers Quarterly Contribution Report (see facsimile — Figure 1). The Contribution Reports are audited for completeness and accuracy, and then key-punched. Each Contribution Report contains the following identification:

1. A four-digit Standard Industrial Classification (S.I.C.) Code
2. A three-digit area code designating the county or city in which the reporting establishment is physically located
3. A six-digit serial or identification number unique to each establishment

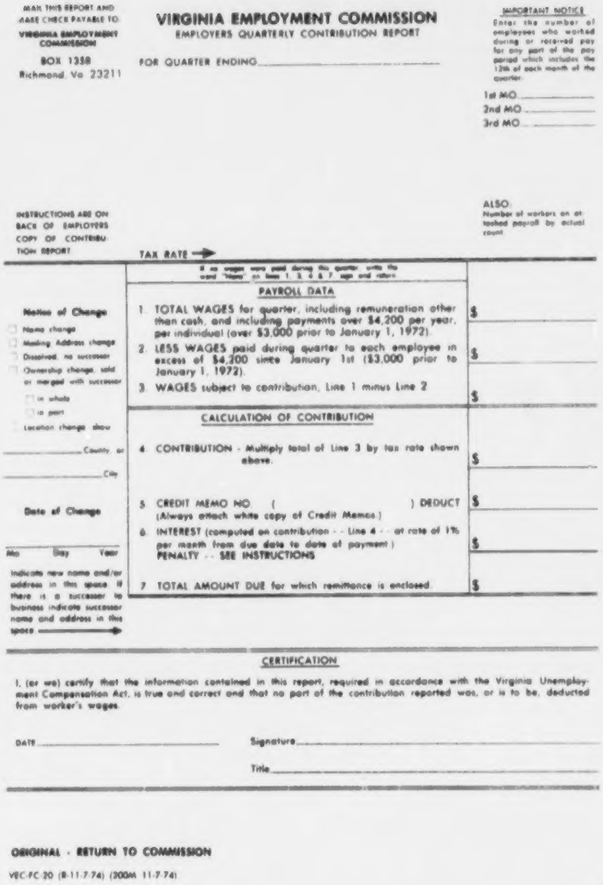
As was mentioned, U.I. Contribution Reports are filed quarterly and contain (in Virginia) the following data:

1. Monthly Employment
2. Gross Quarterly Payroll
3. Gross Quarterly Payroll subject to Unemployment Insurance
4. Quarterly contribution, i.e., U.I. tax
5. Quarter and year liability (to U.I.) started
6. Report date (quarter and year)

MANUFACTURING DATA

Of these items above, employment (item #1) and gross quarterly payroll (item #2) are of particular importance to the water resource planner. Payroll is of special relevance, since when cumulated by quarter to an annual figure it is a major component of value-added. This index, value-added, has been and is currently used extensively as an economic indicator (past, present and future) of water-use and waste generated. The U.I. payroll in manufacturing is also an important component of gross manufacturing output or value-of-product.

Figure 1. Contribution Report



MAIL THIS REPORT AND
MAKE CHECK PAYABLE TO
VIRGINIA EMPLOYMENT
COMMISSION
BOX 1358
Richmond, Va 23211

VIRGINIA EMPLOYMENT COMMISSION
EMPLOYERS QUARTERLY CONTRIBUTION REPORT

FOR QUARTER ENDING ____________

IMPORTANT NOTICE
Enter the number of employees who worked during or received pay for any part of the pay period which includes the 12th of each month of the quarter.

1st MO. ________
2nd MO. ________
3rd MO. ________

ALSO:
Number of workers on attached payroll by actual count

INSTRUCTIONS ARE ON BACK OF EMPLOYERS COPY OF CONTRIBUTION REPORT

TAX RATE →

If no wages were paid during this quarter, write the word "None" on lines 1, 3, 4 & 7, sign and return

Notice of Change
☐ Name change
☐ Mailing Address change
☐ Dissolved, no successor
☐ Ownership change, sold or merged with successor
☐ in whole
☐ in part
☐ Location change, show
________ County or
________ City

Date of Change
____
Mo Day Year

Indicate new name and/or address in this space. If there is a successor to business indicate successor name and address in this space →

PAYROLL DATA

1. TOTAL WAGES for quarter, including remuneration other than cash, and including payments over $4,200 per year, per individual (over $3,000 prior to January 1, 1972).	$
2. LESS WAGES paid during quarter to each employee in excess of $4,200 since January 1st ($3,000 prior to January 1, 1972).	$
3. WAGES subject to contribution, Line 1 minus Line 2	$

CALCULATION OF CONTRIBUTION

4. CONTRIBUTION - Multiply total of Line 3 by tax rate shown above.	$
5. CREDIT MEMO NO. ( ) DEDUCT (Always attach white copy of Credit Memos.)	$
6. INTEREST (computed on contribution - - Line 4 - - at rate of 1% per month from due date to date of payment.) PENALTY - - SEE INSTRUCTIONS	$
7. TOTAL AMOUNT DUE for which remittance is enclosed.	$

CERTIFICATION

I, (or we) certify that the information contained in this report, required in accordance with the Virginia Unemployment Compensation Act, is true and correct and that no part of the contribution reported was, or is to be, deducted from worker's wages.

DATE ____________
Signature ____________
Title ____________

ORIGINAL - RETURN TO COMMISSION

VEC-FC-20 (R-11-7-74) (200M 11-7-74)

As a prerequisite for access to the E.S. 202 — U.I. data, it is necessary that the requesting agency be aware of the publication restraints and data non-disclosure requirements. In Virginia the publication criteria are as follows:

1. The industry group must include at least three independent reporting firms (i.e., companies — not establishments).
2. The industry's employment must be sufficiently dispersed so that the combined employment of the two largest firms does not exceed 80 per cent of the group total.
3. Individual firm data may not be published or disclosed verbally under any circumstances.
4. E.S. 202 data may not be used for law enforcement purposes, except in the administration of the U.I. law under which the data is required.

In most states, other detailed economic data germane to water resource planning is available in both published and unpublished form. In many instances, the unpublished data by firm or reporting establishment is an extremely flexible planning tool. The data usually has been collected by reporting unit and contains identification which is similar to and compatible with the U.I. reports discussed above. In Virginia, an Annual Survey of Manufacturers is conducted by the State Department of Labor and Industry. This survey is based on a selected sample and represents about 75 per cent of all manufacturing activity in the State. Firms which participate in the survey are assigned the following identification data:

1. A four-digit Standard Industrial Classification code
2. A three-digit county or city code
3. A five-digit serial or identification number

The Annual Survey of Manufacturing is conducted by a mailed questionnaire referred to as the S-1 form. Questionnaire data items include:

1. Total employment
2. Production worker employment
3. Salaries and wages (total payroll)
4. Wages paid to production workers
5. Net selling value-of-product
6. Cost of materials
7. Contract work
8. Physical volume-of-product
9. Capital expenditures
10. Anticipated capital expenditures
11. Cost and quantity (KWH) of electric power consumed

Value-added is not surveyed directly as a questionnaire item. It can be easily computed, however, as follows:

$$\text{Value-added}=(\text{Net selling value of products})-(\text{Cost of materials})-(\text{Contract Work})$$

The same publication and disclosure restrictions as outlined regarding the E.S. 202—U.I. data apply to the Annual Survey of Manufacturing records, (i.e., S-1 data).

In Virginia, extensive water resource and water quality management plans are being developed for the nine major river basins (see River Basin Map—Figure 2). These studies were begun by the Virginia Division of Water Resources in 1966 and are being completed by the Virginia State Water Control Board (see footnote 1). This planning is being approached in a six volume format.[5] Within Volume II — Economic Base Study, considerable emphasis is placed on the analysis of manufacturing data. This priority reflects the significance of high water-use and related high waste potential of many manufacturing categories.

Much water resource planning is conducted on a hydrologic format. In order to express benchmark manufacturing data on a hydrologic basis, a major rearrangement of E.S. 202 — U.I. data and S-1 data (Annual Survey of Manufacturing) was necessary. This realignment of the data went beyond the normal county and city format. The county and city codes were useful, however, as a broad hydrologic sort routine. As a preliminary step, the punched cards for both the E.S. 202 file and the S-1 file were interpreted and sorted by county and city. Obviously, many counties and cities are completely within the major hydrologic areas. In those counties or cities which are situated in two or more hydrologic areas, however, detailed address determinations of individual firms had to be made. It was necessary, therefore, to have address data for each reporting firm or establishment which was as specific as possible regarding physical location. Usually the firm's mailing address coincided closely with the firm's physical location. Based on this address, a valid hydrologic address determination could be made. This task was especially easy when the firm had an address indicating a physical location well within a particular river basin. The more difficult hydrologic address determinations were those where a firm was located near a ridge line. In these instances, a good deal of map detail was necessary. These "ridge-line" address (hydrologic) determinations could be accomplished by field trip or by correspondence with knowledgeable people within the "ridge-line" locality itself. This latter, less expensive alternative was chosen.

A number of forecasting methodologies[6] (or combinations thereof) are compatible with the data base discussed above. The behavior of price-adjusted, annual payroll data was quite encouraging when subjected to several exponential growth curves. This experience, coupled with the availability and continuity of U.I. payroll data, indicated that growth curve fitting and extrapolation would be fairly valid as a general forecasting technique. Asymptotic growth curves describe an industry passing through the following stages:

1. Period of initial industrial development and limited production — a phase characterized by slow growth
2. Stage of accelerated industrial development, increasing production and rapid expansion
3. Period of relative stability where the growth rate levels off with the main emphasis on operating efficiency and cost minimization

Curves fitted using the Gompertz equation adhered closely to most historical payroll data in the study areas (River Basins and Planning Districts). A Gompertz curve has the shape of a nonsymmetrical "S" when graphed on arithmetic paper. Its nonsymmetrical nature results from a difference in behavior on opposite sides of the points of inflection. The Gompertz equation generates a curve in which the growth increments of the logarithms are declining by a constant percentage. The general equation of the Gompertz curve is:

$$Y_c=Ka^{(bx)}$$

where:

Y_c=Trend value
x =Time interval
K =Asymptote or limit which the trend value approaches as x approaches infinity
a =The distance from the asymptote to the Y-intercept
b =The base of the exponential equal to the constant ratio between successive first differences of the log Y

Two other growth trends which are useful as forecasting equations are the Modified Exponential and the Pearl-Reed (logistic). These equations may be categorized with the Gompertz trend in the broad family of exponential curves. The general equations for the Pearl-Reed and the Modified Exponential may be written as follows:

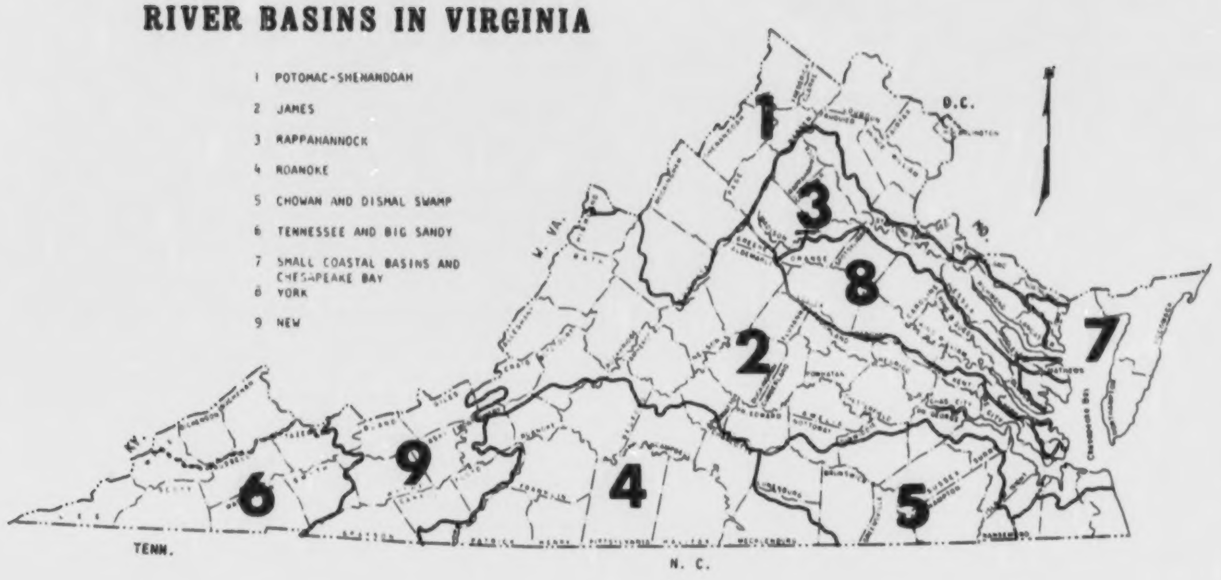
Pearl-Reed	Modified Exponential
$Y_c=\dfrac{K}{1+10^{a+bx}}$	$Y_c=K+ab^x$

---

[5] Volume I - Introduction; Volume II - Economic Base Study; Volume III - Hydrologic Analysis; Volume IV - Water Resource Problems and Requirements; Volume V - Engineering Development Alternatives; Volume VI - Implementation of Development Alternatives.

[6] Other forecasting techniques have utilized standard growth rate tables such as those based on the compound interest rate formula. Industrial projections have also been inferred from predictions of population trends.

Figure 2. Major River Basins in Virginia.



The Pearl-Reed curve traces a pattern in which the first differences of the reciprocals of the Y_c values are declining by a constant percentage. The Modified Exponential curve describes a trend where the amount of growth declines by a constant percentage.

Figure 3 provides an illustration of a typical exponential growth curve. As is evident, the trend line (TT') increases, but at a decreasing rate on the right of the point of inflection. The horizontal line (KK') marks the upper limit of growth or the horizontal asymptote.

Asymptotic growth curves approaching horizontal limits were fitted to the price adjusted U.I. payroll data. Whenever a valid "data fit" was established, an equation resulted. An extension of the curve marked a trend of possible growth. Several growth curves fitted to various intervals of data in the same historical series were used to create a range of projections. Value-added, gross manufacturing output and employment were correlated to payroll data for the forecast reference points.

Prior to growth curve fitting, it is well to look critically at several aspects of the data and the study area:

1. An appraisal should be made to determine if historical growth experience by the industry under study is actually a valid trend.
2. Is the available data record of sufficient length to present a representative trend in the area and industry under study?
3. Is the historical record of sufficient magnitude to represent a data base wide enough to portend future industrial development?

Our experience indicates that price adjusting U.I. Payroll data is an absolute necessity prior to growth curve fitting. Price adjusting, of course, eliminates the fluctuations of inflation or deflation, leaving "real" changes. Unfortunately, there is no "ideal" price index for price adjusting payroll or labor costs.

The Wholesale Price Index[7] (published by the Bureau of Labor Statistics (B.L.S.), U.S. Department of Labor) has proven quite satisfactory when applied to manufacturing payroll data. Most applications have been on the two-digit S.I.C. level using the 1967 base converted to 1970.

The Bureau of Water Resources of the Virginia State Water Control Board now has available 15 years (1956-1970) of U.I. employment and payroll data. An IBM 360 computer is currently being used for the exponential curve fitting routines. Previously, an Olivetti Programma 101 (a programmable calculator) and an IBM 1130 computer were used. The IBM 360 has, of course, greatly expedited curve fitting and extrapolation routines.

Utilizing the "360" program, fifteen years of historical payroll data were fitted to three exponential curves — Gompertz, Modified Exponential and Logistic (Pearl-Reed). The data was analyzed in 6, 9, 12 and

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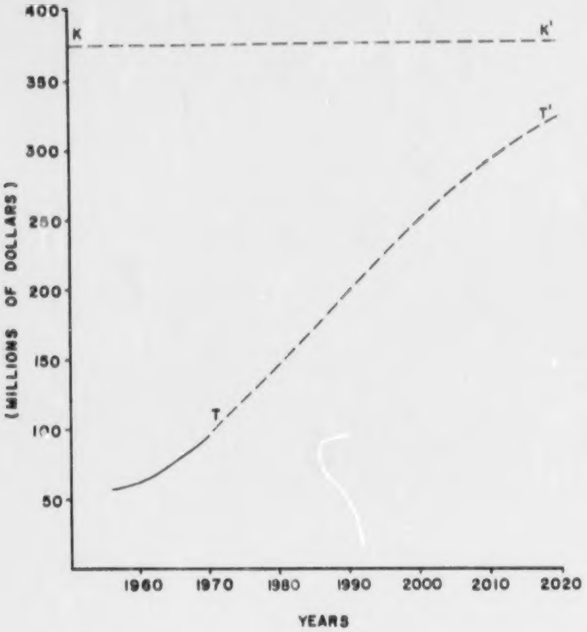
[7] The Wholesale Price Index "...is an index of the prices at the primary market levels where the first important commercial transaction for each commodity occurs." (Tuttle, 1957). 'Wholesale', as used in the title of the index, refers to sales in large quantities, not to prices received by wholesalers, jobbers, or distributors." (U. S. Department of Labor, B.L.S. Handbook, 1971).

Figure 3.
U.I. Payroll estimates and projections in transportation, communications and public utilities for the Southeastern Virginia Planning District (data expressed in constant 1970 dollars).



15-year intervals. For fifteen consecutive years of data, this method resulted in twenty-two possible curve fits for each two-digit S.I.C. Since there were several different forms which the exponential curves could take, constraints were built into the program to eliminate the curves which did not fit a pattern of normal growth. The desired shape of the growth curve was that which sloped upward to the right, approaching some horizontal limit, while increasing at a decreasing rate (see figure 3).

Fifteen years of annual payroll data (1956-1970) were read in for each industry. The first six-year period (1956-1961) was analyzed, and the exponential equation was developed. If the equation did not violate the built-in constraints, then the program extrapolated the historical data from the initial year of the fit period (in this case 1956) to the year 2020. If the equation violated the constraints, a message was printed out indicating that there was no fit for that series. The second group of consecutive years of payroll data (1957-1962) was then analyzed. This continued through the twenty-two possible combinations until the final serial (1956-1970) had been analyzed.

The extrapolated universe payroll values, payroll-per-employee, S-1 value-added, S-1 gross manufacturing output and S-1 payroll were used in a Programming Language 1 (PL1) program which generated a table of projections for value-added, gross manufacturing output, payroll and employment. The tables were structured for photographic reproduction directly from the printout, thus eliminating virtually all typing and proofing. The value-added projections were developed by computing the ratio of S-1 payroll and S-1 value-added for the benchmark year. This ratio was applied to the extrapolated payroll figures to develop the universe value-added projections. The gross manufacturing output projections were developed in much the same way. The ratio of S-1 payroll to S-1 gross manufacturing output was computed for the benchmark year, and this was applied to the extrapolated payroll values to give gross manufacturing output projections. The extrapolated payroll values were divided by the extrapolated payroll-per-employee figure to develop employment projections for each S.I.C. group.

Because of the large volume of output from the exponentials, another method of analysis has been devised which expedites the evaluation of the extrapolations. A curve plotting routine has been added to the exponential programs so that each curve that extrapolates is also graphed. This enables the analyst to pick the best fit from the plots without having to analyze reams of computer print-outs. A FORTRAN IV[8] program has been written to utilize the plotter capability of the IBM 360. This plotter routine will graph the price-adjusted historical payroll data and all possible extrapolations. By employing transparent plotting paper and a uniform scaling factor, an overlay effect is created for the graphic extrapolations within each S.I.C. The three exponentials -- Gompertz, Pearl-Reed and Modified Exponential -- are thereby grouped and the trend selection process is greatly facilitated. A clustering effect is a "reasonable" indication of a medium range projection.

A COBOL[9] routine is used at this point to expand the extrapolated U.I. payroll to a universe. This universe payroll figure will include U.I. payroll, B.O.A.S.I. payroll and non-covered payroll. Universe employment data can then be estimated by dividing the universe payroll projections by extrapolations of payroll-per-employee. Value-added and gross manufacturing output (Value-of-product) can be projected through correlation of benchmark payroll to value-added and payroll to gross manufacturing output (G.M.O.).

POPULATION STATISTICS

In Virginia, the Division of State Planning and Community Affairs (D.S.P.C.A.) has been designated as the agency responsible for the State's population projections. This Division (D.S.P.C.A.) has recently published population forecasts for all counties and cities in Virginia. These projections are on an every ten year basis to the year 2020.

The planning guidelines of the Virginia Division of Water Resources required a range of population forecasts. The range of projections (high, medium and low) reflect varying demographic assumptions. The low projections assume a very subdued rate of industrial development and continued out-migration of the resident population. The medium forecast is based on a rather vigorous industrial development program.

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[8] FORTRAN IV is a computer language which is used most frequently in scientific and engineering applications. The term FORTRAN relates to the primary use of the language: FORmula TRAnslating.

[9] COBOL is a computer language which is used extensively in business and commercial data processing. The term COBOL is derived from the expression COmmon Business Oriented Language.

An extremely accelerated rate of economic growth is implicit in the high projection. High and low projections were generated by fitting the compound interest rate formula above and below the D.S.P.C.A. forecast (medium). This trend fitting was accomplished using a FORTRAN IV program on an IBM 1130 computer. County and city population projections developed by the Virginia Division of State Planning and Community Affairs were used by the Division of Water Resources as the medium range on which the high and low projections were based.

The following high and low control totals (in thousands) were assumed for the entire state:

Virginia Population (X1000)

	1970	1980	1990	2020
High		5,632	6,919	12,100
(Medium)	4,648	5,415	6,284	9,340
Low		5,198	5,629	7,100

The average annual rate of change was computed for each ten-year period using the compound interest rate formula:

$$\text{Average annual rate of change} = R = \sqrt[n]{\frac{X_t}{X_1}} - 1$$

e.g. X_t = 5,629,000 - 1990 State low
X_1 = 5,198,000 - 1980 State low
n = 10 (years)
R = 0.00799

A set of ten constants were then computed, five high (H_i) and five low (L_i). These can be defined for each ten-year period as the differences between R for the high projection (RH_i) and R for the medium (RM_i), and the difference between RM_i and for the low (RL_i):

$$H_i = RH_i - RM_i \qquad i = 1,5$$
$$L_i = RM_i - RL_i \qquad i = 1,5$$

These constants were then applied to each county and city in developing the high and low projections.

RC_i was computed for each county and city for each ten-year period, using D.S.P.C.A.'s medium projections:

$$RC_i = \sqrt[n]{\frac{X_t}{X_1}} - 1$$

For a given county or city, then, the high projections were computed as follows:

$$Hi(1980) = (1970\ \text{Popl'n})\ (1.0 + H_1 + RC_1)^{10}$$
$$Hi(1990) = Hi\ (1980)\ (1.0 + H_2 + RC_2)^{10}, \text{etc.}$$

and the low:

$$Lo(1980) = (1970\ \text{Popl'n})\ (1.0 - L_1 + RC_1)^{10}$$
$$Lo(1990) = Lo\ (1980)\ (1.0 - L_2 + RC_2)^{10}, \text{etc.}$$

BITUMINOUS COAL MINING

An analysis of Virginia's bituminous coal mining industry was made in Volume II — Economic Base Study of the Tennessee and Big Sandy River Basins. Three basic economic indicators — production, employment and productivity — were presented. Production in the coal industry is measured in mine tonnage and has experienced an increasing trend in Virginia since the late 19th century. Record keeping has been quite good in this industry and a comprehensive set of historical data[10] is available from the Virginia Department of Labor and Industry. Based on the availability and continuity of this data, growth curve fitting and extrapolation were selected as reasonable forecasting techniques.

Asymptotic growth curves describe a mineral industry passing through the following stages:

1. Period of initial exploration, market development and limited production, a phase characterized by slow growth
2. Stage of sharply increasing production and rapid expansion
3. Period of relative stability where the growth rate levels off with the main emphasis on operating efficiency and cost minimization

The three exponential curves (Gompertz, Pearl-Reed and Modified Exponential) discussed on the above pages were used in this analysis.

The medium range projection represented the rates of growth believed to be the most probable. High and low projections were also developed. These three forecasts provided a range of data wherein certain water resource planning alternatives could be tested.

Basically the same approach (asymptotic growth curves) was used to project the future low employment trend in the coal industry. Because of the historically declining employment series, a low range curve with a negative trend and a lower limit was fitted and extrapolated.

CURRENT PROJECTS

Recent emphasis in Virginia has been on Metropolitan/Regional Plans to the State's Water Quality Management Plan. The Metropolitan/Regional Plans are being developed for Virginia's twenty-two planning districts. Since the planning districts are aggregations of entire counties and cities, the data base, described above, was arrayed and manipulated using the three-digit county or city codes. The basic economic parameters developed in the river basin plans, discussed above, were also generated for the Metropolitan/Regional Plans.

Data has recently been developed for a special water quality management study for the lower James River Basin. The project (The Lower James River Basin Comprehensive Management Study), often referred to as the "3c" Study, was authorized under Section 3(c) of the 1965 Federal Water Pollution Control Act. The purpose of the 3(c) Study is to develop a viable water quality management plan for one of the most intensively developed sections of Virginia's largest river basin.

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[10] Annual Reports, Virginia Department of Labor and Industry, 1951-69

The data assembled for the "3c" Study includes standard parameters for all industries and follows a county and city format. Economic data for the "3c" Study was generated in terms of a 1970 benchmark and ten-year projections to the year 2020. Those indexes requiring price adjustments were expressed in constant 1970 dollars.

The forecasting methodology for the "3c" Study data generally paralleled the techniques discussed regarding the manufacturing data. Again, extrapolations of "growth curves" fitted to price adjusted payroll data were correlated to other parameters such as employment and sales. The major exception was in a shift from the B.L.S. Wholesale Price Index to the B.L.S. Consumer Price Index for price adjusting historical payroll data. The "3c" Study places considerable emphasis on "real" income of the Study area in relation to the proposed expenditures for water quality management. Payroll data (for all industries) price adjusted with the Consumer Price Index should produce a fairly realistic indication of how local income can meet expenditure recommendations. Certain non-payroll data, however, such as manufacturing value-added, gross manufacturing output and wholesale trade receipts was adjusted with the Wholesale Price Index.

CONCLUSIONS

Economic data adds an important dimension to water resource and water quality management planning. Payroll and employment statistics collected to administer State Unemployment Insurance programs have a multitude of applications in economic analysis and forecasting. U.I. data is a continuous, carefully maintained and relatively extensive set of historical records. It has been accumulated under national guidelines of the U. S. Department of Labor, Manpower Administration and is quite uniform in format. U.I. records have, for years, been structured for data processing applications. Further manipulation of this data such as price adjusting and trend fitting are thus facilitated. Most of the standard economic parameters of water resource and water quality management planning such as value-added and gross manufacturing output have been correlated to U.I. payroll and employment benchmarks. The Annual Survey of Manufacturing (Virginia Department of Labor and Industry) provides value-added and gross manufacturing output data. County and city detail and a data processing format is an important feature of the Annual Survey (S-1). Both the U.I. and S-1 data have been further formated by hydrologic area in Virginia. On balance, the U.I. and S-1 data have become valuable tools for water resource and water quality management planning in Virginia.

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MODELING RADIATIVE TRANSFER IN THE PLANETARY BOUNDARY LAYER: PRELIMINARY RESULTS

Francis S. Binkowski, NOAA*

Meteorology and Assessment Division
Environmental Sciences Research Laboratory
Environmental Research Center
Research Triangle Park, N.C. 27711

Abstract

Long wave radiative fluxes and cooling rates are calculated using a statistical band model. The vertical quadratures are sums of analytic integrals of the transmission functions. The calculated cooling rates and fluxes compare very favorably with observations.

Introduction

The prediction of pollutant dispersion conditions in the lower troposphere for use in air quality simulation models requires information about the temperature profile, since atmospheric thermal stability strongly influences the character of dispersion. Thus, the problem becomes to predict the temperature profile in a realistic way. One of the major influences on the temperature profile especially at night, but also in the late afternoon is the rate of change of the net long wave (infrared) flux with height (or pressure).

This paper will discuss a method for calculating the upward, downward and net fluxes for clear skies (no clouds) and clean air (no aerosol) cases. When methods for treating clouds and aerosol are introduced into the calculation method, comparisons with the benchmark case (clear skies- clean air) as well as with real atmospheric data will be possible.

Many methods have been proposed for calculating these fluxes. The most flexible methods are those which divide the terrestrial spectrum into finite intervals and calculate the transmission of infrared radiation within each spectral interval and sum over the contributions of each interval. Atwater (1966), Rodgers and Walshaw (1966), Ellingson (1972) and Fels and Schwartzkopf (1975) have all used this method. All these authors also used a random band model for the transmission function. That is, the transmission for each spectral interval was obtained by considering the absorption lines within the spectral interval to be randomly spaced and to have intensity specified by some probability distribution. The random band model approach is used here as well as a transmission function model which has a more realistic probability distribution for water vapor (Malkmus, 1967) and has a simpler mathematical form than previous transmission models. This transmission function has not been used for this purpose in the open literature before.

Since our interest is in the lower troposphere, we shall consider only those absorbers which are most important in this part of the atmosphere. Thus, water vapor and carbon dioxide are the only absorbers considered. Ozone which has a strong absorbtion band at 9.6μ, and is in the water vapor "window" of 8 to 13 μ was not considered in the present work. The quantitative effects of this ommission are unknown since real-time tropospheric ozone profiles were unavailable for the comparisons discussed below. Qualitatively, the most important effect of ignoring ozone is that the downward flux at the surface is smaller than it would be if ozone were considered. Ozone will be added in future calculations. All other gases present in trace amounts are also ignored. As mentioned previously, the band model approach used here is flexible enough to permit additional absorbers to be treated relatively easily. Other absorbers will be considered when it becomes apparent from comparison with measurements that it's necessary to include them.

Method of Calculation

We start with the equation of radiative transfer in integrated form is given by Rodgers and Walshaw (1966)(with slight modification)

$$\downarrow F(z)=B(z)+\{\downarrow F(H)-B(H)\}T(U_t)+\int_0^{U_t} \frac{dB}{du'}(u')T(u')du' \quad (1a)$$

$$\uparrow(F(z)=B(z)+\{\uparrow F(g)-B(0)\}T(U_b)+\int_0^{U_t} \frac{dB}{du'}(u')T(u')du' \quad (1b)$$

where for each spectral interval $\downarrow F(z)$, $\uparrow F(z)$ and $B(z)$ are respectively the downward, upward and blackbody fluxes at the reference level z and $\downarrow F(H)$, $\uparrow F(g)$ and $B(0)$ are respectively, the downward flux at the top of the computational domain H, the upward flux at the ground, g, and the blackbody flux at the bottom of the atmosphere. The definite integrals are taken over the amount of absorber (water vapor) u' between z and levels above z in (1a) and between z and levels beneath z in (1b). The total absorber amounts from z to H and from z to the ground are U_t and U_b respectively. The transmission function $T(u')$ is defined such that $T(0) = 1$ and $T \to 0$ as $u' \to \infty$. The integral

$$I = \int_0^U (u')T(u')du'$$

may be written without approximation as the sum

$$I = \sum_{i=1}^{n} \int_{U_{i-1}}^{U_i} \frac{dB}{du'}(u')T(u')du'$$

where U, which may represent U_t or U_b has been divided into n increments $\Delta u \equiv u_i - u_{i-1}$. If we represent $dB(u')/du'$ by an average value for each increment of Δu such that

$$\frac{dB}{du'} \doteq \frac{B(u_i) - B(u_{i-1})}{\Delta u} \equiv \frac{\Delta B}{\Delta u}$$

then

$$I \doteq \sum_{i=1}^{n} \frac{\Delta B}{\Delta u} \int_{u_{i-1}}^{u_i} T(u')du' \quad (2)$$

Both of the definite integrals in (1) may be approximated in this way. This approximation of dB/du' by $\Delta B/\Delta u$ is strictly valid only when B varies linearly over u'. In practice only discrete values of B and u' are available, either from radiosonde measurements in the atmosphere or from grid point calculations. The approximation in (2) says that between these discrete values B varies linearly with u'. This is the simplest approximation which allows B to vary between levels. This may be viewed as a next step from considering an isothermal slab between the discrete points. The approximation is invoked in order to obtain the form (2) which contains the integral of the transmission function, T, over absorber amount u'. If the precise form of T specified is analytically integrable, then the definite integrals in (1a,b) may be given by simple sums.

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* On assignment from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce

We shall use the transmission function of Malkmus (1967) discussed by Rodgers (1967):

$$T(u') = \exp\{-a(1+bu')^{\frac{1}{2}} + a\} \tag{3a}$$

which may be integrated as

$$\int_{u_{i-1}}^{u_i} T(u')du' = 2a^{-1}b^{-2}\{(Y_i-a-1)\exp(Y_i)-(Y_{i-1}-a-1)\exp(Y_{i-1})\} \tag{3b}$$

where $Y_i = -a(1+bu_i)^{\frac{1}{2}} + a$, and the parameters a and b to be discussed below, are held constant. Thus the approximation dB/du' by ΔB/Δu, combined with (3b) indicates a simple efficient computation scheme.

The band parameters a and b are defined by (Rodgers, 1967) as

$$a = \frac{\pi\alpha}{2\delta}\overline{p} \quad , \quad b = \frac{4k}{\pi\alpha\overline{p}}$$

or for notational convenience

$$a = \hat{a}\overline{p} \quad , \quad b = \frac{\hat{b}}{\overline{p}}$$

where k, α, and δ are respective by average line intensity, half width (at one atmosphere) and line spacing which are representative of the spectral interval considered; and $\overline{P}$ is an average pressure (discussed below) for the layer defined by Δu. The expressions $\hat{a}$, $\hat{b}$ may be obtained from the wave length, half width and intensity of individual spectral lines within each interval. Rodgers and Walshaw (1966) discuss the use of line data for determining $\hat{a}$, $\hat{b}$, and also recommend the use of the Curtis-Godson approximation to correct the $\hat{a}$, $\hat{b}$ for changes in temperature and pressure along an atmospheric path. This approximation defines a corrected absorber amount $\overline{u}$, and a mean pressure $\overline{P}$ between two levels say i, j as:

$$\overline{u}(i,j) = \sum_{\ell=i}^{j} \int_{P_{\ell-1}}^{P_\ell} 1.66\,\phi r\,\frac{dp}{g} \tag{5a}$$

$$\overline{P}(i,j) = \frac{1}{\overline{u}(i,j)} \sum_{\ell=i}^{j} \int_{P_{\ell-1}}^{P_\ell} \psi\left(\frac{P}{P_{oo}}\right) r\,\frac{dp}{g} \tag{5b}$$

where r is the mixing ratio, P is pressure, P_{oo} is 101.325 kPa and 1.66 is the diffusivity factor for calculating the diffuse fluxes from beam transmission functions (Armstrong, 1969; Ellingson, 1972). The φ and ψ functions are obtained by calculating values of $\hat{a}$, $\hat{b}$ at three temperature values and fitting empirical functions of the form (Rodgers and Walshaw, 1966):

$$\phi(\theta) = \exp\{A(\theta-\theta_o) + B(\theta-\theta_a)^2\} \tag{6a}$$

$$\psi(\theta) = \exp\{A'(\theta-\theta_o) + B'(\theta-\theta_o)^2\} \tag{6b}$$

This representation recovers values of $\hat{a}$, $\hat{b}$ within the temperature range considered with a relative error of 1% or less. The line data of McClatchey et. al., (1973) were used to calculate $\hat{a}$,$\hat{b}$,A',B' with a reference temperature θ_o of 275K. With values of A, B, A', B' (6) may be used in (5) to evaluate the corrected absorber amount $\overline{u}$, and mean pressure $\overline{p}$. Then, if the corrected absorber amount is used as the variable of integration in (3b), with $\overline{p}$ constant for each layer, a and b are constant for the integration. The temperature and pressure effects are included in the ΔB/Δu term through the factor $2a^{-2}b^{-1}$ in (3b), thus Δu is an increment of corrected absorber amount. The six calculated band parameters were favorably compared with Rodgers and Walshaw (1966) for consistency where possible. The line data of McClatchey et.al., however, includes information which was not available to Rodgers and Walshaw (1966). This procedure was used to calculate the transmission function for water vapor for intervals from 0-760cm^{-1} and 1200-2500cm^{-1}.

The 8-13μ window was treated differently. The absorption in this spectral region is of somewhat different character than that treated previously. The absorption appears as a "continuum" (Bignall, 1970), that is a region of nearly constant absorption. The transmission function may be given as

$$T = \exp\{-K_s U\}$$

where K_s is a constant and u is a corrected absorber amount defined as

$$u(i,j) = \sum_{\ell=i}^{i} \frac{1}{P_{oo}} \int_{P_{\ell-1}}^{P_\ell} 1.66(0.005P + 0.995e)\,\hat{\phi}\,r\,\frac{dp}{g}$$

where the pressure, p, term represents the broadening of the individual lines by collision with other species, and the water vapor pressure, e, term represents self broadening by water vapor (Bignall, 1970; McClatchey et.al., 1972). The temperature correction term

$$\hat{\phi} = \exp\{1745/\theta - 5.90\}$$

is an empirical correction term due to Lee (1973). When corrected absorber amount u is used as a variable of integration, this transmission function may be analytically integrated. This transmission function and its integral were used for the two intervals 760-1000cm^{-1} and 1000-1200cm^{-1}.

Carbon dioxide is treated in a highly parameterized way. For one spectral interval 560-760cm^{-1}, which includes the entire 15μ CO_2 band an empirical transmission function due to Rodgers and Walshaw (1966) is used. This transmission function, T(c), is also integrable in terms of the carbon dioxide amount c. The overlap of CO_2 and water vapor for the one spectral interval 560-760cm^{-1} is treated by calculating a mean transmission $\overline{T}$ given by

$$\overline{T} = \frac{1}{c_i - c_{i-i}} \int_{c_{i-1}}^{c_i} T(c)\,dc$$

where C_i is the carbon dioxide amount at the same level as U_i. The water vapor transmission functions in (3) are then multiplied by $\overline{T}$ in the integrals and by T(C) where C is the total CO_2 above or beneath z as appropriate. This parameterization is used for two reasons: first, it seems to yield good results in comparisons with cases when no CO_2 is used; second, it is simple, efficient, and economical compared with a more comprehensive scheme such as used by Fels and Schwartzkopf (1975) in which a detailed line by line integration is used. A band model approach for CO_2 such as used by Ellingson(1972) is quite costly since he used 15 intervals for the CO2 alone and the present model only considers 12 intervals in total.

Planck functions, B, were calculated by a Gauss-Laguerre numerical quadrature scheme due to Johnson and Branstetter (1974). A simple 5 point formulation gave 6 decimal place accuracy, which is certainly sufficiently accurate for the present needs. This is to be contrasted with the 96 point Gaussian quadrature of Ellingson (1972) which also gave 6 place accuracy.

As mentioned above, 12 intervals were used. This is to be compared with 20 intervals used by Rodgers and Walshaw (1966); 125 intervals used by Atwater (1966) and 100 intervals used by Ellingson (1972). Calculations with as many as 18 intervals were indistinguishable from calculations with 12 intervals, but calculations with 7 intervals were markedly poorer, especially in the calculated cooling rates as compared with observed cooling rates. Only results from the 12 interval model will be presented here.

Equations (1a,b) together with approximations (2a,b) and the appropriate transmission functions are used to calculate the upward and downward fluxes. The downward flux at the top is taken to be blackbody flux times an emissivity of 0.01 which gives the right order of magnitude for the downward flux at 20 kPa. The bottom surface, at present, is taken to have an emissivity of 1.0. The cooling rates are obtained from the divergence of the net flux, that is

$$\frac{\partial T}{\partial t} = - \frac{1}{\rho C_p} \frac{\partial F_n}{\partial z} = \frac{g}{C_p} \frac{\partial F_n}{\partial p}$$

where F_n is the net flux ($F_n = \uparrow F - \downarrow F$). At present, the vertical p-derivative is approximated by a finite difference.

Results of Validation Calculations

To assess the validity of the method of calculation the clear skies measurements discussed by Gille and Kuhn (1973) were used for comparison with calculations presented here. Temperature and mixing ratio at 5 kPa (50mb) increments from 100 to 20 kPa were used as input data. Upward, downward and net fluxes were calculated at the input levels and compared with the *in situ* measurements of Gille and Kuhn. Results of this comparison are shown in Figure 1. The *in situ* data shown are from over water ascents of the U.S. Radiometer-sonde in the vicinity of Panama on four clear skies evenings (0000GMT ± 20 minutes). Figure 1 displays the means of the measurements and the means of the calculations for the upward, downward and net calculations, while Figure 2 displays the means of the measured and calculated cooling rates. Visual inspection of the figures indicates a good correspondence between observations and calculations. Table 1 shows "student t" values (Weatherburn, 1961) for the comparison of these means. The table indicates that for 5% significance level with 3 degrees of freedom ($t=3.18$) the means do not differ for any of the fluxes or cooling rates. The interpretation is that a set of sample calculations is indistinguishable from a set of measurements. This is consistent with the findings of Gille and Kuhn (1973) who used results of Ellingson's (1972) model for calculations.

A somewhat more demanding test of model performance is a comparison of case by case predictions for the clear skies cases. The relative error of the calculation compared with the observation, (OBSERVED-CALCULATED)/OBSERVED, for each case was calculated and averaged. A perfect model would have this average relative error equal to zero. The "t" values for this comparison are displayed in Table 2, where we see that four values are significant at the 5% level. The lowest three altitudes of downward flux and the lowest value of the net flux. The relative error for the downward flux are of the order of 8%, while the relative error of the net flux is quite large because of the small value of the flux.

We may compare these errors to the differences that exist among simultaneous measurements. Gille and Kuhn (1973) show comparisons of the U.S. radiometer-sonde with a German and a Japanese instrument. For the 90 kPa altitude there was a 2% difference in downward flux between the U.S. measurement and the mean of all three (U.S., German, Japanese), which is significant at the 5% level. Further the model calculations of Ellingson used by Gille and Kuhn showed an underestimate of the order of 5% for the same altitudes. These differences are also significant at the 5% level ($t \sim 4.0$). Gille and Kuhn also give some tentative evidence of a systematic overestimate of downward flux and systematic underestimate of net flux by the U.S. radiometer-sonde when compared with surface measurements from a Linke-Feussner instrument. Thus the errors, that is, differences between the observed and calculated fluxes, taken on a case by case basis are real and significant, but of the same order of magnitude as differences among radiometer-sondes, and of the same order of magnitude as other calculations.

The cooling rate differences show no significant difference at the 5% level between calculations and measurements. This is encouraging, since the cooling rate is the dynamical variable needed for prediction of the temperature profile.

Conclusions

The 12 interval model presented here is capable of calculating useful estimates of the upward, downward and net fluxes and cooling rates in the lower troposphere for the clear skies, clean air case.

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TABLE 1 The t values for comparison of mean of calculations with mean of measurements for upward, downward, and net fluxes and the cooling rates.

Pressure (kPa)	Upward	Downward	Net	Cooling rate
100	0.35	2.21	-3.04	1.52
90	2.47	1.04	-1.29	0.06
80	1.81	1.27	-0.99	0.28
70	1.73	1.36	-0.97	0.71
60	1.82	0.47	-0.66	0.91
50	1.65	0.68	-0.26	0.62
40	1.25	0.55	0.06	1.13
30	0.58	0.22	-0.27	0.95
20	0.35	0.29	0.61	1.89

Negative value indicate an over-estimate in the calculations.

TABLE 2 The t values for relative error of calculation compared with measurements on a case by case basis for upward, downward, and net fluxes and the cooling rates.

Pressure (kPa)	Upward	Downward	Net	Cooling rate
100	1.09	6.55*	-3.83*	1.25
90	3.00	5.56*	-2.35	-0.44
80	3.02	3.96*	-1.69	0.05
70	1.56	2.69	-1.81	0.47
60	1.86	1.91	-1.16	0.29
50	1.81	0.84	-0.68	-1.17
40	1.39	0.88	-0.08	1.33
30	0.81	0.20	0.35	1.11
20	0.80	-1.78	0.93	-0.09

* Significant at the 5% confidence levels for 3 degrees of freedom. t= 3.18

FIGURE 1

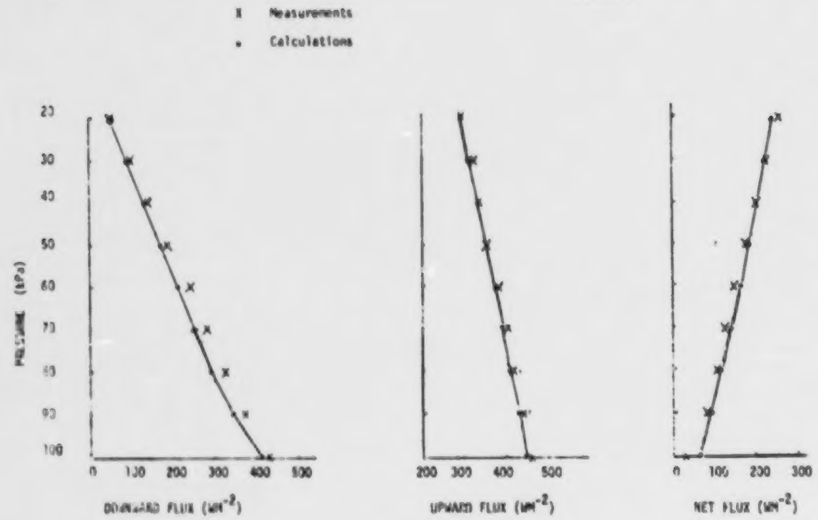

Figure 1 : Comparison of mean measured with mean calculated fluxes for upward, downward, and net fluxes.

FIGURE 2

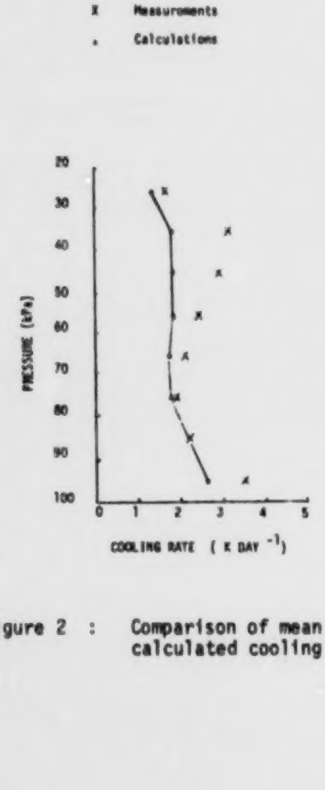

Figure 2 : Comparison of mean measured and mean calculated cooling rates.

ADAPTIVE FORECASTING OF BACKGROUND CONCENTRATIONS USING FEEDBACK CONTROL AND PATTERN RECOGNITION TECHNIQUES

R. Carbone
Academic Faculty of Management Sciences
The Ohio State University
Columbus, Ohio

W.L. Gorr
School of Public Administration
The Ohio State University
Columbus, Ohio

Abstract

This paper develops and tests an empirically-based model for tracking and forecasting background concentrations of air pollutants. A set of variables (e.g., meteorological, locational, economic activity levels, etc.) and a functional form relating the variables constitute the model. The technique for estimating the parameters of the model is derived from recent developments in adaptive feedback and pattern recognition. Time-varying characteristics of the parameters are "tracted"; and thus, automatically adapted to structural changes in the air pollution system. The model and estimation technique are applied to total suspended particulates background in Allegheny County, Pennsylvania, as a pilot test.

1. Introduction

The clean air program for attainment and maintenance of air quality standards (AQS's) has given rise to a number of modeling requirements for the time series of pollutant concentrations. (See Rhoads [1] for a concise review of programs.) Program planning for regulation of pollutant emissions, capacity expansion, facilities location etc. requires models relating control variables to the controllable component of air quality. These models are common; see for example [2], [3], and [4]. In addition, it is necessary to model the uncontrollable component in order to obtain total or ambient concentrations. Planning tends to involve special, "once only" studies in a decision process that yields a regulated time series of concentrations designed to fall within target levels.

Program evaluation of plans and their implementation requires, on the other hand, routine modeling of the time series for tracking, detection of disparities with targeted levels, diagnosis of cause, and correction. Large numbers of variables and massive quantities of data are involved in the clean air program so that a staged modeling approach is desirable with the early stages being automated and suggestive of the later, specialized stages.

Tracking models should provide robust and up-to-date estimates of ambient concentrations so that significant changes can be detected. Such models may also form the basis for simple forecasts through extrapolations of the tracked time series. If there is a disparity between current or forecasted concentrations and targeted levels, then it is required to advance to a second stage of automated modeling for preliminary diagnostics.

First, tracking and forecasting should be extended to separate the controllable and uncontrollable components of the time series to determine which is the problem. Second, a sufficient number of explanatory variables (e.g., meteorological, economic activity level, regulatory activity level etc.) should be correlated to concentrations through multivariate statistical models so that analysts can theorize as to the causes of the problem. From this basis, analysts could proceed if necessary to a third stage of analysis which would be non-routine and involve further measurements, experiments, or other special studies. The results of diagnostic work would serve the decision process for modifications of plans or targets.

This paper presents an approach, the adaptive statistical diffusion model (ASDM), which is promising for many of the program requirements outlined above. The ASDM is a multivariate time series model based on a "time-varying parameters" principle and feedback estimation procedures leading to a highly flexible and automated modeling capability. Section 2 formulates the ASDM and its estimation procedure, and Section 3 provides program applications. Sections 4 and 5 give a specific application to total suspended particulates (TSP) background in Allegheny County (Pittsburgh), Pennsylvania. Finally, Section 6 outlines future work.

2. Adaptive Estimation and Forecasting of Pollutant Concentration Over Time: a General Approach

2.1 Model Formulation

The ASDM consists of a set of explanatory variables and time-varying parameters combined in a functional form for pollutant concentrations. An important aspect of the ASDM is that all parameters are assumed to be time-varying, and in the estimation procedure discussed below, parameter estimates are updated sequentially as each observation of the explanatory variables occurs. This leads to the potential for automatically capturing the effects on concentration of missing variables and system structural changes. For example, suppose an air pollution source to the west of a concentration monitor has major impacts on the monitor, but pollutant emission strength is a missing variable. If wind direction (from which the wind blows) sectors are represented by a set of indicator variables, then the time-varying parameter for the variable "west" might account for effects on concentration of trends or cycles in emissions.

The explanatory variables can be arbitrarily classified as "quantitative" which refers to dimensioned quatities such as wind speed, or "qualitative" which leads to 0/1 indicators for nominal classes of the qualitative variable; e.g., north, east, south, and west for wind direction; no, mild, and heavy for precipitation. A general first-order equation presented in [6] portrays a useful interaction phenomenon between quantitative and qualitative variables in a time-varying framework. Applied to the air pollution problem, this becomes the ASDM:

$$y(t) = \prod_{i=1}^{m} \alpha_i(t)^{z_i(t)} \left[\sum_{j=1}^{n} \beta_j(t) x_j(t) \right] + u(t) \qquad (1)$$

$$t = 1,2,\ldots$$

where a specific averaging time, pollutant species, and point p in geographic region R are assumed; and

$y(t)$ = pollutant concentration at time t,
$z_i(t)$ = the i-th qualitative indicator which takes values of 0 or 1 depending on

whether or not the i-th nominal class occurs at t,

$\alpha_i(t)$ = the parameter for the t-th observation associated with the i-th qualitative indicator,

$x_j(t)$ = the t-th observation for the j-th quantitative variable,

$\beta_j(t)$ = the parameter for the t-th observation associated with the j-th quantitative variable, and

$u(t)$ = an undefined error term.

A normalization process is employed for the qualitative variables: one nominal class, a "$z_j(t)$" indicator, is suppressed in the ASDM for each qualitative variable; e.g., "north" for wind direction and "no precipitation" for precipitation. The collection of suppressed nominal classes for all qualitative variables becomes the "standard" qualitative condition. An observation of this standard would then result in the value of 0 for all remaining, non-standard $z_i(t)$'s in the product portion of the ASDM. Thus the product would take the value 1 and the ASDM for the standard condition would simply be:

$$y(t) = \sum_{j=1}^{n} \beta_j(t)x_j(t) + u(t) \tag{2}$$

Observations with non-standard conditions result in a product greater or less than 1 reflecting the relative effect on the standard concentration model as in (2).

2.2 Estimation Algorithm

Our purpose is to obtain updated estimates of the $\alpha(t)$ and $\beta(t)$ parameters for each observation in order to capture and track the changing effects of the variables on concentration. Due to the nature of our problem, the algorithm used should possess certain desirable properties:

a. It should be designed to minimize over-reactions to pollutant measurement and other transient errors, and thus, provide robust estimators.

b. Estimates of the parameters should be updated without requiring any a priori knowledge of the kind of processes which may govern their time variation. This aspect is crucial since changes in uncontrollable conditions that may occur in the future are seldom known or accurately predicted in advance.

c. From an operational point of view, the high rate of observations occurring over time requires the use of an algorithm which involves sequential processing of information as opposed to batch processing. It should be computationally tractable and implementable on widely available computers.

An approximation method for estimating time-varying parameters, Adaptive Estimation Procedure (AEP), recently developed by Carbone and Longini, see [5] and [6], lends itself to the nature of our formulation and problem. In this methodology, robust time-varying estimators are generated without using any a priori knowledge by recursively updating values via the following two formulas:

$$\hat{\beta}_j(t) = \hat{\beta}_j(t-1) + |\hat{\beta}_j(t-1)| \left[\frac{y(t) - \hat{y}(t)}{\hat{y}(t)} \cdot \frac{x_j(t)}{\bar{x}_j(t)} \cdot \frac{1}{D}\right] \tag{3}$$

for all $j = 1,\ldots,m$

and

$$\hat{\alpha}_i(t) = \hat{\alpha}_i(t-1) + \hat{\alpha}_i(t-1) \left[\frac{y(t) - \hat{y}(t)}{\hat{y}(t)} \cdot z_i(t) \cdot \frac{1}{\ell D}\right] \tag{4}$$

for all $i = 1,\ldots,n$

where $\hat{y}(t)$ = predicted concentration for time t based on $\hat{\beta}(t-1)$ and $\hat{\alpha}(t-1)$ estimators,

D = damping parameter > 1,

ℓ = the number of qualitative variables (or groups of nominal indicator variables), and

$\bar{x}_j(t)$ = updated average for the j-th quantitative variable.

An exponential smoothing scheme is used to calculate this latter average as follows:

$$\bar{x}_j = S_0 x_j(t) + (1-S_0)\bar{x}_j(t-1)$$

where $0 < S_0 < 1$

3. Applications

The problem of attainment and maintenance of AQS's is to determine values of control variables (e.g., fuel quality, emission-control-device efficiences, stack heights, etc.) affecting the controllable component of concentration, $C_p(t)$, so that

$$A_p(t) = C_p(t) + B_p(t) < \delta_p(t) \text{ for all p in R} \tag{5}$$

where $A_p(t)$ = total or ambient concentration averaged over a period of specified length (e.g., a year) ending at t,

$C_p(t)$ = controllable component,

$B_p(t)$ = background component, and

$\delta_p(t)$ = AQS.

In order to calculate estimates or forecasts of $A_p(t)$ and its components, it is necessary to average the ASDM estimate, y(t), over the relevant period by calculating simple averages, or by developing a joint probability distribution of all explanatory variables for calculating expected values as done in [2] and [3]. Several approaches have been used or proposed for constraints (5); from maximum technically feasible controls [7], to satisficing with some tradeoffs in cost versus air quality achievement [8], and to cost-effectiveness [9], [10].

An estimate, $\hat{A}_p(t)$, of ambient concentration is obtainable through samples at any p through the ASDM. For remote regions, R_r, with no significant controllable sources of pollutants, it is reasonable to assume that concentration is uniform over p but not t; i.e.,

$$\hat{A}_p(t) = \hat{A}_{p*}(t) \text{ for all p in R} \tag{6}$$

where p* is the location of any properly mounted monitor in R_r. It is also common to assume that model (6) provides an estimate for background concentration occurring in developed or urban regions R_u (see [11]):

$$\hat{B}_q(t) = \hat{A}_{p*}(t) \text{ for all } q \text{ in } R_u \tag{7}$$

Thus the ASDM has direct use for tracking, forecasting, and diagnosing concentrations through models (6) and (7) using concentration samples from p*.

For attainment, the federal AQS's are a constant over p and t; i.e., $\delta_p(t) = \delta$. However, proposals for maintenance of air quality have the following definition [12]:

$$\delta_p(t) = A_p(1974) + \gamma_p(t) \tag{8}$$

where $\gamma_p(t)$ is a specified series of allowable increments of degradation of air quality. If the region is rural, then model (6) suffices for $\delta_p(t)$. If the set of urban monitoring sites is extensive or representative of air quality, then $\hat{A}_p(t)$ as modeled by the ASDM for all available monitoring sites may be sufficient for $\delta_p(t)$. Interpolation may be required between monitoring sites.

Background concentration is often estimated as the concentration advected into R_u as sampled by "background monitors" located at the boundaries of R_u; see, for example, Pooler [13], Rubin and Bloom [14], and Samson *et al.* [15]. Here the ASDM extends the concept of a pollution rose (see Munn [16]) where background is identified by the wind directions corresponding to advection into R_u. Sections 4 and 5 develop the ASDM background model in detail; where for example, one model is

$$\hat{B}_p(t) = \hat{B}_{d*}(t) \text{ for all } p \text{ in } R_r \tag{9}$$

where d* represents a dummy site. This "site" is a composite of all background monitor sites such that only samples from wind directions corresponding to advection are utilized.

For program evaluation purposes, it is possible to estimate the controllable, or more accurately, the local component of concentration by difference:

$$\hat{C}_p(t) = \hat{A}_p(t) - \hat{B}_p(t) \tag{10}$$

where $\hat{A}_p(t)$ and $\hat{B}_p(t)$ are estimated by the ASDM approach. In this way, tracking and forecasting may reveal the effects of controls by separating out background.

4. A Demonstration

We now focus our attention on an empirical study to demonstrate and test out the ASDM approach. The study is mainly directed at forecasting and tracking changes in total suspended particulate (TSP) background concentration over time in Allegheny County, Pennsylvania. It involves the analysis of some 800 observations of daily average particulate concentration recorded from 1970 to 1975 at two monitors located at opposite boundaries of the county. The location of the two "background" monitors chosen and surrounding major point sources is found in a map of the county presented in Figure 1.

In addition to daily average particulate concentration monitored (by hi-vol) by the Allegheny County Bureau of Air Pollution Control, six variables were used in the study to reflect meteorological and structural conditions. They are the 24 hour resultant wind direction, average wind speed, precipitation, inversion; and finally, two factors reflecting general activity level, weekend or weekday and cooling or heating day. Information on these various conditions for each observation were obtained from the U.S. Department of Commerce, Local Climatological data for the Greater Pittsburgh Airport and the Denardo & McFarland Weather Services, West Mifflin, Pennsylvania.

The next task was to determine how to enter the variables into the ASDM structure. Both inversion and wind speed were defined as quantitative aspects; whereas, the remaining were considered as qualitative. Here, only a ground level inversion of strength greater than 2°C determined an inversion, which corresponds to air-pollution-emergency "watch" conditions in Allegheny County. Also, the inverse of average wind speed was the measure utilized. Wind direction was broken down into eight classes (0-45 degrees, 45-90 and so on) and precipitation into four (no precipitation; low, 0-.10 inches; mild, .10-.35 inches; and heavy, .35 and over). Having identified the predictors and how to incorporate them, the study then proceeded according to the following steps.

step 1: a third input file, herein referred to as Monitor III, containing only observations with background wind directions (315-360 and 0-135 degrees for Monitor I and 135-315 degrees for Monitor II) was created.

step 2: AEP was applied to the three sets of input data in the following way.

a. The initial value for all the parameters was set equal to 1.
b. A standard qualitative condition was defined as weekend, cooling day, 315-360 degrees resultant wind direction, and no precipitation. This implies that the parameters associated with these characteristics were held equal to 1 when running the procedure.
c. $S_0 = .04$ was used for updating mean values for the quantitative aspects.
d. A dampling parameter of D = 50 was initially assumed and subsequently readjusted

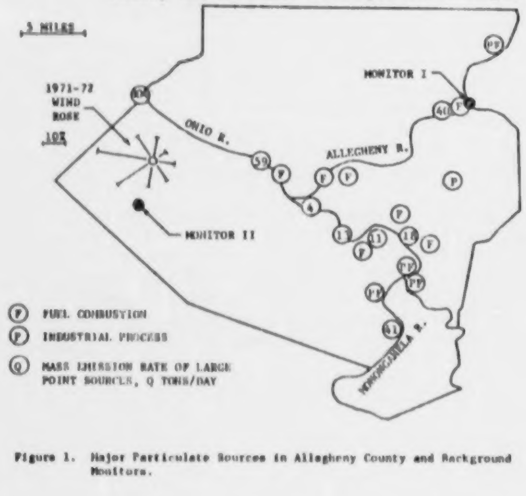

Figure 1. Major Particulate Sources in Allegheny County and Background Monitors.

via a recycling procedure (see [6]). The recycling of the observations was necessary here because of the small number of observations over the years covered (370 for Monitor I, 410 for Monitor II, and 411 for Monitor III), so as to converge to experienced patterns of change.

5. Results

Some descriptive measures of predictive performance of ASDM are presented in Table 1. The measures contained in the table are first, average actual ($\overline{AC}$) and predicted ($\overline{PC}$) concentration, and also their standard deviations, (SAC) and (SCP). The table further contains the root mean square prediction error (RMSPE), the simple correlation coefficient (r) between predicted and observed values, the mean absolute percentage deviation (MAPD), and the serial correlation coefficient (ρ) of a first-order autoregressive scheme.

By carefully examining Table 1, we observe that the results are promising in terms of the RMSPE, r, and MAPD; and comparable to diffusion modeling results of others (see for example, Slade [17] p. 142, McCollister and Wilson [18], and Bankoff and Hanzevack [19]). The ASDM results have little or no error in central tendency detected; and also, we note no evidence of first-order serial correlation in our results for the three monitors. What may appear somewhat disturbing is that the standard deviation of the predicted concentrations is consistently smaller than for the observed values. However, it can easily be argued that because of the expected large measurement errors present in TSP data, the spread of true concentration should be smaller than that of observed concentration. The AEP is specifically designed to track true measurements (see [6]) rather than observed values.

Table 2 presents ASDM parameter estimates for Monitor I at two points in time--the start and end of the five year study period. Attention is focused on this monitor since it has had the greatest degree of time-variation in the parameter estimates. The values in Table 2 give results as theoretically expected; for example, the results reveal that concentration on a weekday is about 24% greater than on weekends at the beginning of the period and 12% at the end which provides some measure of the general effectiveness of control policies; that a low precipitation level reduces concentration by approximately 12% in contrast to no precipitation over the period; that a resultant wind direction from the major point sources (225-270 degrees) located next to the monitor (see Figure 1) leads to about 79% greater concentration than the standard direction assumed which is of a background nature; and that total concentration given the standard qualitative condition assumed for no-inversion-high-wind-speed days decreased from 68 $\mu g/m^3$ to 50 $\mu g/m^3$.

A value of 35 $\mu gm/m^3$ annual geometric mean for TSP background was assumed for Allegheny County in the 1971 state implementation plan. More recently, the U.S. EPA assumed a 1972 value of 30 $\mu gm/m^3$ falling to 20 $\mu gm/m^3$ between 1975 and 1980; and Rubin and Bloom [14] estimated 45 to 50 $\mu gm/m^3$ based on a pollution rose of Monitor II (1971-72). Thus, TSP background has been found to be a significantly large component of ambient TSP air quality in Allegheny County. Our estimates show, however, that the background component is even larger than in the previous estimates.

Figure 2 presents two plots of expected total concentration using Monitor III weights (background monitor). The plots presented illustrate the acute TSP background problem in Allegheny County: under the con-

Table 1

Some Descriptive Measures of ASDM Performances

	Monitors		
	I	II	III
$\overline{AC}$	86.81	67.35	65.74
$\overline{PC}$	88.10	69.64	66.95
SAC	43.34	36.26	35.68
SPC	32.98	21.94	18.83
RMSPE	33.49	32.65	32.64
r	.6458	.4622	.4194
MAPD	34.33	33.97	35.77
ρ	-.124	.020	-.001

Table 2

ASDM Parameter Estimates for Monitor I: Start and End of Period.

Variables	Percent or Mean Value	Parameter Estimate Start	End	Variables	Percent or Mean Value	Parameter Estimate Start	End
Degree Day				Wind Direction			
Heating	28.11	0.859	0.842	00 - 45	4.05	0.760	0.744
Cooling	71.89	1.000	1.000	45 - 90	5.41	0.931	0.931
Day				90 - 135	8.65	0.845	0.853
Weekend	26.22	1.000	1.000	135 - 180	7.57	1.342	1.259
Weekday	73.78	1.249	1.127	180 - 225	10.27	1.539	1.576
Precipitation				225 - 270	34.32	1.796	1.773
None	43.51	1.000	1.000	270 - 315	17.30	1.410	1.328
Low	20.27	0.881	0.855	315 - 360	12.43	1.000	1.000
Mild	15.95	0.841	0.813	Wind Speed^{-1}	0.12	53.08	46.79
Heavy	10.27	0.926	0.907	Inversion	30.00	7.98	18.57
				Constant	1.00	67.59	49.91

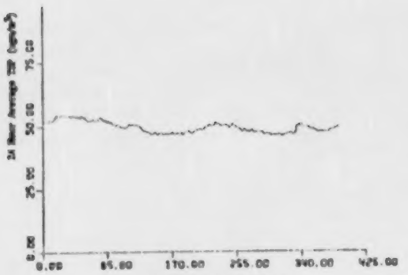

Figure 2(a). Wind Direction from 0-45°.

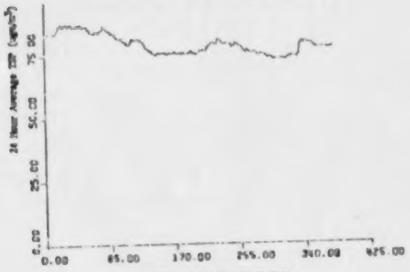

Figure 2(b). Wind Direction From 225-270°.

Figure 2. ASDM Time Series of TSP Concentration for Monitor 111 and the Conditions: Cooling, Weekday, No Precipitation, No Inversion, and 10 miles/hour Wind Speed.

ditions specified, there is a nearly constant trend of high background concentration. This observation is consistent with the fact that the updated mean TSP background over all conditions computed via an exponential smoothing scheme varied from 75 μgm/m^3 at the beginning of the period to 68 μgm/m^3 at the end. It appears, from current evidence, that attainment of the federal secondary annual TSP standard of 60 μgm/m^3 is impossible regardless of local control policies.

6. Future Work

It is desirable to model a pollutant sampled more frequently and with a short averaging time than the case in this paper. It appears that a 24 hour averaging time provides overly aggregated data with respect to variation in the underlying phenomenon. In future work, it is also desirable to further investigate the functional form used in the ASDM; e.g., as to which variables should be multiplicative, transformed etc. Finally, we wish to pursue the relationship of adaptive modeling to the decision framework of the clean air program, and to determine the requirements of the decision maker.

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SOURCE-ORIENTED EMPIRICAL AIR QUALITY MODELS[*]

Kenneth L. Calder
Environmental Protection Agency
Environmental Sciences Research Laboratory
Research Triangle Park, N.C.

William S. Meisel
Technology Service Corporation
Santa Monica, CA. 90403

ABSTRACT

Meteorological dispersion functions in multiple-source simulation models for urban air quality are usually specified on the basis of the analysis of data from special field experiments, usually involving isolated sources. In the urban environment, individual sources cannot be isolated. One may, however, ask for a source-receptor relationship which, when summed (or integrated) over all the sources, would minimize the average squared error in prediction of measured values. The feasibility of this approach is demonstrated by application to model-generated data, where the source-receptor relationship is known.

INTRODUCTION

In commenting on the lack of acceptance of empirical/statistical models in air quality modeling in 1973, one of the authors called attention to "the historical belief that air quality models based on statistical regression type of analysis are not source-oriented and, therefore, are largely useless for control strategy in terms of the contribution of individual sources to the degradation of air quality"[1]. He went on to ask "whether, with an appropriate analysis, a source-oriented statistical-type of air quality model could be developed which did not involve prior specification of meteorological dispersion functions per se and incorporation of these as in present air quality models. My thought here is that for given 'meteorological conditions' these dispersion functions play the role of transfer functions between the air quality distribution and the distribution of pollutant emissions, and if one were smart enough might, therefore, conceivably be obtained empirically by a mathematical inversion technique (as, for example, by numerical solution of sets of integral equations) utilizing accumulated data on the distributions of air quality and emissions. If this could be accomplished then maybe a major shortcoming of the current statistical models could be removed and we should then in effect have an alternative to the customary meteorological-dispersion type of modeling." These comments suggest the motivation for the study reported[2].

The difficulties in developing a source-oriented empirical model can be stated from a statistical point of view. The spatial distribution of pollutant concentrations over a region is determined by emissions and meteorological conditions. The number of variables determining the concentration at a given point is tremendous, particularly since emissions arise from a large number of point sources and area sources. Consequently the number of emission variables alone can easily be in the hundreds. If an empirical model were to be developed in the most obvious manner, there should be an attempt to relate the pollutant concentration at a given point to all the possible emission variables and meteorological variables affecting the concentration at that point. Since the determination of the relationship between emission/meteorological variables and concentration requires examples of that relationship over a very wide range of emission and meteorological variables, a tremendous amount of data would be required to adequately determine this relationship.

If we could, however, isolate a given emissions source and we had a number of receptor locations scattered about the source, the variation in wind speed and direction would cause a wide variation in measured concentration at the receptor locations. With enough examples of the source-receptor relationship, the variation of the concentration with distance from the point source could be determined empirically.

In the urban environment, of course, individual sources cannot be isolated. Measurements are the result of contributions from a number of sources. However, because of the wide diversity of meteorological conditions, the concentration will vary widely at a given point, and the sources which contribute to the concentration at that point will similarly vary. One may then ask for a consistent source-receptor relationship which, when summed (or integrated) over all the sources, would explain best on the average the observed concentrations. More specifically, one could choose the source-receptor function which minimized the average squared error in prediction of the measured values. This concept is the core of the ideas tested.

The data used to test these ideas are model-created data. Model data were chosen for three major reasons:

1. With model data, the source-receptor function is known and can be compared with the function extracted from the data. With measurement data, "truth" is unknown.

2. Area sources and point sources can be isolated and studied separately as well as jointly.

3. The cost of verifying and organizing measurement data would have been beyond the scope of the present study.

MATHEMATICAL FORMULATION

We work with a rectangular coordinate system with x-axis along the mean horizontal wind direction, with y-axis crosswind, and with the z-axis vertical. Then in urban air quality models it is customary to consider the pollutant emissions in terms of a limited number (say J) of elevated point-sources together with horizontal area-sources, the latter being possibly located at a few distinct heights ζ_s (say, for example, for $s = 1,2,3$). The total concentration $\chi(x,y,0)$ at ground level at the receptor location $(x,y,0)$ will be the sum of the concentration contribution from the point-source distribution, say $\chi_P(x,y,0)$ and that from the area-source distribution $\chi_A(x,y,0)$, i.e.,

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$$\chi(x,y,0) = \chi_p(x,y,0) + \chi_A(x,y,0) \qquad (1)$$

where

$$\chi_p(x,y,0) = \sum_{\ell=1}^{J} Q_p(\ell)K(x-\xi_\ell,y-\eta_\ell;0,\zeta_\ell) \qquad (2)$$

$$\chi_A(x,y,0) = \sum_{s=1}^{3} \iint_A Q_A(\xi,\eta,\zeta_s) \cdot K(x,\xi,y-\eta;0,\zeta_s)d\xi d\eta \qquad (3)$$

and

$Q_p(\ell)$ = emission rate of ℓ-th elevated point-source, located at position $(\xi_\ell,\eta_\ell,\zeta_\ell)$

$Q_A(\xi,\eta,\zeta_s)$ = emission rate of horizontal area-source distribution located at height ζ_s, and A denotes the total integration domain of the area-source distribution

$K(x-\xi,y-\eta;0,\zeta)$ = source-receptor function; it gives the ground level concentration at the receptor location $(x,y,0)$ resulting from a point-source of unit strength at (ξ,η,ζ).

Note that this formulation includes the assumption of horizontal homogeneity, namely, that the impact of a given source upon a given receptor depends only upon their relative and not absolute coordinates. This assumption is true for an urban environment only in an average sense. A single wind direction is similarly valid only in an average sense. Finally, it should be noted that the above formulation assumes steady-state conditions and is thus only applicable for relatively short time periods (of the order of one hour), when this may be an adequate approximation providing the emissions and meteorological conditions are not rapidly changing.

In equations (2) and (3) above it is convenient to use "source-oriented" position coordinates, and to consider a typical ground-level receptor location as (x_i,y_i), $i=1,2,\ldots$.

Let

$$x' = x_i-\xi \ , \quad dx' = -d\xi \ , \quad x'_{i\ell} = x_i-\xi_\ell \qquad (4)$$
$$y' = y_i-\eta \ , \quad dy' = -d\eta \ , \quad y'_{i\ell} = y_i-\eta_\ell$$

Then

$$\chi_p(x_i,y_i,0) = \sum_{\ell=1}^{J} Q_p(\ell)K(x'_{i\ell},y'_{i\ell};\ 0,\zeta_\ell) \qquad (5)$$

$$\chi_A(x_i,y_i,0) = \sum_{s=1}^{3} \iint_A Q_A(x_i-x',y_i-y',\zeta_s) \cdot K(x',y';0,\zeta_s)dx'dy' \qquad (6)$$

In the following several different source-receptor functions $[K(x',y';0,\zeta)]$ will be considered, including the classical Gaussian form that is the basis for the RAM-model [3]. For the latter, and with the meteorological condition of infinite mixing depth

$$K(x',y';0,\zeta) = \frac{\exp\left\{-\frac{y^2}{2\sigma_y^2(x')}\right\}\exp\left\{-\frac{2}{2\sigma_z^2(x')}\right\}}{\pi U\ \sigma_y(x')\sigma_z(x')} \ . \qquad (7a)$$

where U denotes the mean wind speed, and we assume simple power-law dependencies for the standard deviation functions, say

$$\sigma_y(x') = a_y(x')^{b_y} \qquad (7b)$$

$$\sigma_z(x') = a_z(x')^{b_y}. \qquad (7c)$$

Also, as in the RAM-model we will assume that the narrow-plume hypothesis may be employed in order to reduce the double integral of equation (6) to a one-dimensional integral. Thus, under this hypothesis, if

$$\int_{-\infty}^{\infty} K(x',y';0,\zeta_s)dy' = G(x',\zeta_s), \qquad (8)$$

then in place of equation (6) we have

$$\chi_A(x_i,y_i,0) = \sum_{s=1}^{3} \int_{x'} Q_A(x_i,x',y_i,\zeta_s)G(x',\zeta_s)dx' \qquad (9)$$

which only involves values of the area-source emission rates in the vertical plane through the wind direction and the receptor location.

For the special case of a Gaussian plume

$$G(x',\zeta_s) = \sqrt{\frac{2}{\pi}}\ \frac{\exp\left\{-\frac{\zeta_s^2}{2\sigma_z^2(x')}\right\}}{U\sigma_z(x')} \qquad (10)$$

The basic equations (5) and (6) (or (5) and (9)), with the Gaussian forms for $K(x',y';\ 0,\zeta)$ and $G(x',\zeta)$ involve four unspecified parameters through the equations (7b) and (7c), namely, a_y,b_y,a_z and b_z. More generally, any functional form chosen for K (and therefore G) may have unspecified parameters; we will denote the set of unspecified parameters by the vector $\underline{\alpha}$. Thus for the special Gaussian form

$$\underline{\alpha} = (a_y,b_y,a_z,b_z) \qquad (11)$$

The explicit dependence of the calculated concentration values on these parameters could be indicated by the notation $\chi(x_i,y_i,0;\underline{\alpha})$.

The basic method employed in this study is that of choosing $\underline{\alpha}$ to minimize the error between calculated and observed values of concentrations.* In order to express this statement formally, we must elaborate our notation to indicate explicitly the dependence on wind direction; thus $\chi(x_i,y_i,0;\theta;\underline{\alpha})$. For each wind direction $\theta_j(j=1,2...R)$ there is a concentration observation for each receptor location (monitoring station). The receptor locations are denoted (x_i,y_i) for $i=1,2...N$, and are assumed to be at ground level so that we may omit the symbol 0 in the χ-notation. Then the mean square error over all observations is

$$e^2(\underline{\alpha}) = \frac{1}{RN}\sum_{i=1}^{N}\sum_{j=1}^{R}\left[\chi_{obs}(x_i,y_i,\theta_j)-\chi_{calc}(x_i,y_i;\theta_j;\underline{\alpha})\right]^2$$

$$= \frac{1}{RN}\sum_{i=1}^{N}\sum_{j=1}^{R}\Big[\chi_{obs}(x_i,y_i;\theta_j)-\chi_p(x_i,y_i;\theta_j;\underline{\alpha})$$

$$-\chi_A(x_i,y_i;\theta_j;\underline{\alpha})\Big]^2 \qquad (12)$$

where χ_p and χ_A are given by Eqs. (5) and (6) (or (5) and (9)).

The problem of minimizing e^2 with respect to $\underline{\alpha}$ is a standard optimization problem. Chambers provides a good recent survey of available techniques[4]. The particular technique we employed was "structured random search"[5]; this is a rather inefficient technique, but one which does not require calculation of derivatives and which converges under difficult conditions (given enough time). This technique's main advantage was that we could modify the form of the source-receptor function without modifying the search technique. The results of applying this methodology to the best data are discussed following; however, we first turn to a description of the test data.

TEST DATA

For a realistic distribution of point-sources, area-sources and receptor locations, use was made of unpublished information from a 1968 air pollution study conducted in St. Louis, Missouri[6]. The area sources were gridded into over 600 square regions; there were 60 point sources and errors were calculated at 40 receptors for the 16 wind directions. (See Reference [1] for more details.) The corresponding concentration data were generated by the EPA-developed RAM algorithm[3], which is a specific implementation of the classical Gaussian plume formulation, that considers both point- and area-sources, with three possible heights for the latter, and which uses the "narrow-plume" hypothesis (i.e., Eq. (9)) to calculate the area-source concentration contribution χ_A. A constant wind speed U of 5 meters per second was employed, and sixteen wind directions at the points of the compass were simulated. Infinite mixing depth and a neutral atmospheric stability category were assumed. For the latter, in Eqs. (7b) and (7c), we have

$$\begin{aligned} a_y &= 0.072 \quad , \quad b_y = 0.90 \\ a_z &= 0.038 \quad , \quad b_z = 0.76 \quad . \end{aligned} \qquad (13)$$

For this data, these values and the indicated equations are optimal and would produce zero mean-square error. It is this result we hope to be able to recover from the data by the optimization procedure.

OPTIMIZING PARAMETERS FOR THE GAUSSIAN FORM OF THE SOURCE-RECEPTOR FUNCTION

The data base described earlier contains concentration values at forty receptors and sixteen wind directions, a total of 640 values (referred to as "actual" values). The contribution to the concentration from point and area sources was available separately, as well as in toto.

Equations (5) and (7a) provide a prediction of the point-source pollutant concentration at any given receptor location once the four parameters are specified. A comparison of values predicted by these equations versus actual values allows calculation of the root-mean-square value of the error with a given choice of parameter values. (See Eq. (12), with area sources at zero.)

With initial guesses of $a_y=a_z=0.1$ and $b_y=b_z=1.0$, the search routine described arrived at values of

$$a_y = 0.74,\ b_y = 0.92,\ a_z = 0.039,\ b_z = 0.77$$

when the "true" values (those used to create the data) were

$$a_y = 0.72,\ b_y = 0.90,\ a_z = 0.38,\ b_z = 0.76.$$

The root-mean-square (RMS) error initially was 157 $\mu g/m^3$ and the maximum error over the 640 values was 1205 $\mu g/m^3$; the parameter values after 100 iterations yielded an RMS error of 14 $\mu g/m^3$ and a maximum error of 175 $\mu g/m^3$. (Table 1 summarizes these results.) To place the size of the final error in perspective, we note that the actual values (due to point sources alone) were as high as 1545 $\mu g/m^3$.

Employing Eq. (9) for area sources and using only the area-source contribution in the "actual" data, we get similarly promising results (Table 2). Actual values of concentrations due to area sources reach maximums of over 800 $\mu g/m^3$.

The results of treating point and area sources simultaneously, representative of the case which would be encountered with measurement data, are listed in Table 3; the algorithm once again closely approaches the optimum values in 100 iterations. Actual values of the total concentrations from both point and area sources go above 1600 $\mu g/m^3$.

While the initial parameter values we chose in these cases converged toward the values used in creating the data, experimentation indicated that this was not always the case. Small RMS errors could be achieved with combinations of parameters significantly different in value from those used in creating the data. As indicated in Figure 1, rather different combinations of a and b yield very similar values of ax^b over the range of x in which we are interested. It is clear that an essentially equivalent combination of values should not be deemed erroneous, since they yield an accurate empirical model. We regard this a characteristic of the formulation chosen for calculating σ and do not regard it a difficulty of the methodology proposed. Further, in practice, initial values for the parameters would be chosen from the literature, and the solution obtained would be a set of values similar to the initial values, but which minimized the prediction error.

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* "Observed" in the present case is model-created test data; the technique is, of course, intended for practical use on measured data.

Table 1. Point sources only; parameter values at initial, mid, and final iteration during search. (Windspeed is fixed at 5.0 m/sec.)

Iteration	a_y	b_y	a_z	b_z	RMS Error (μg/m^3)	Max. Error (μg/m^3)
0 (initial)	0.100	1.00	0.100	1.00	157	1205
50 (mid)	0.049	0.85	0.050	0.71	85	711
100 (final)	0.074	0.92	0.039	0.77	14	175
ACTUAL VALUES:	(0.072)	(0.90)	(0.038)	(0.76)	(0)	(0)

Table 2. Area sources only; parameter values at initial, mid, and final iteration during search. (Windspeed is fixed at 5.0 m/sec. Values a_y and b_y do not affect area source values.)

Iteration	a_z	b_z	RMS Error (μg/m^3)	Max. Error (μg/m^3)
0 (initial)	0.100	1.00	157	1205
50 (mid)	.028	0.89	15	69
100 (final)	.037	0.79	6	24
ACTUAL VALUES:	(0.038)	(0.76)	(0)	(0)

Table 3. Point and area sources together; parameter values at initial, mid, and final iteration during search. (Windspeed is fixed at 5.0 m/sec.)

					Both Point and Area Sources	
Iteration	a_y	b_y	a_z	b_z	RMS Error (g/m^3)	Max. Error (g/m^3)
0 (initial)	0.100	1.00	0.100	1.00	157	1205
50 (mid)	0.055	0.79	0.044	0.67	79	583
100 (final)	0.074	0.89	0.036	0.74	24	194
ACTUAL VALUES:	(0.072)	(0.90)	(0.038)	(0.76)	(0)	(0)

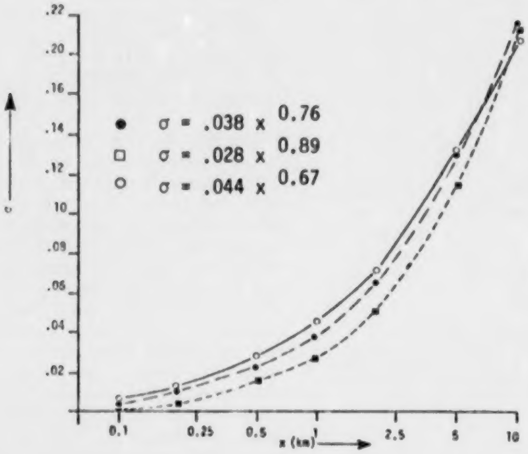

Figure 1. Plot of ax^b for several values of a and b. (The variable x is plotted on a log scale.)

This aspect of implementation also suggests that a good initial guess would be employed and, thus, that convergence to an "optimum" solution would be rapid.

Forty receptors (i.e., air quality monitoring stations) are more than are available in many monitoring systems. How many stations are required for this methodology to be effective? The answer to this question is heavily dependent on the number and distribution of sources, but the indications from experiments with our test data suggest that a considerably smaller number of stations may suffice. Table 4 indicates errors due to changes in parameter values, one at a time, from the optimum values, for a selection of the individual stations. The errors are sufficiently large that one would expect that optimum parameter values could be extracted from a small number of stations at well-chosen locations.

MORE GENERAL SOURCE-RECEPTOR FUNCTIONS

More complex source-receptor functions (such as multivariate polynomials and piecewise quadratic functions) were tested with success[1], but broad conclusions about alternative forms will not be forthcoming through the analysis of the present test data. Analysis of measurement data may allow meaningful comparison of the Gaussian and more general parameterized forms.

CONCLUSION

A methodology for empirically testing alternative forms and extracting optimal parameters for source-receptor dispersion functions has been described. Feasibility was demonstrated on data for which the "true" source-receptor function was known; the methodology recovered parameter values very close to true values. This approach shows promise as a means for calibrating Gaussian-form models for particular urban environments and in testing alternative forms.

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Table 4. Sensitivity Analysis. Root-mean-square and maximum error due to change in each parameter from nominal values at selected receptors. Concentrations are from both point and area sources.

Parameter	Change	Receptor No.	Error (in $\mu g/m^3$) at Selected Receptors.														Error for All 40 Receptors	
			1		10		13		21		22		24		35			
	From	To	RMS	MAX	RMS	MAX	RMS	MAX	RMS	MAX	RMS	MAX	RMS	MAX	RMS	MAX	RMS	MAX
a_y	.072	.079	9	32	67	260	17	46	10	32	11	33	14	52	44	175	16	175
b_y	.90	.99	15	59	23	63	22	69	20	62	20	66	10	31	46	175	24	234
a_z	.038	.042	24	49	32	102	24	45	27	51	16	52	33	109	47	177	27	151
b_z	.76	.836	32	66	44	111	29	62	37	80	23	69	27	65	52	178	35	230
U	5.0	5.2	15	25	18	30	19	44	18	33	16	39	14	37	45	177	18	177

EPA FLUID MODELING FACILITY

Roger S. Thompson and William H. Snyder*
Meteorology and Assessment Division
Environmental Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, N.C.

Summary

A meteorological wind tunnel and a water channel-towing tank as used by EPA scientists for laboratory studies of air pollution dispersion in the vicinity of buildings and over complex terrain are described. In these fluid modeling studies, simulated atmospheric boundary layer flow patterns are created over specially constructed scale models of structures or geographic areas. Modeling theory provides similarity criteria to ensure that flow behavior in the model simulates real processes in the atmosphere. Visualization of dispersion from modeled emission sources is obtained by releasing an oil fog in the wind tunnel and dye in the water channel. Simulated pollutant concentration levels are determined by emitting a tracer, which is sampled and measured at locations of interest around the model site. Neutral atmospheric conditions are modeled in the wind tunnel and in the water channel-towing tank in the recirculating mode of operation. Dispersion under thermally stratified atmospheric conditions is modeled by filling the water channel-towing tank with stratified layers of salt water and towing models through the motionless fluid. Results of some recent projects are presented as examples of the types of information gained at the Fluid Modeling Facility.

Introduction

In-house research in fluid modeling of atmospheric dispersion is conducted at the Environmental Protection Agency's Fluid Modeling Facility (FMF) located in Research Triangle Park, N.C. The FMF, which is a part of the Meteorology and Assessment Division of the Environmental Sciences Research Laboratory, opened in June 1974 with the installation - including instrumentation, shop equipment, and a minicomputer - of the meteorological wind tunnel[1] (Figure 1). In a major expansion of the facility, the installation of a water channel-towing tank (Figure 2) was completed in December 1975.

Fluid modeling involves placing a scale model of a topographic region or an urban area, for example, in a moving fluid to simulate meteorological effects at the site. In a towing tank, the model is moved through motionless fluid. By following scaling laws, full scale atmospheric flow can be accurately simulated in the laboratory. In addition, quantitative measurement of the concentrations of a tracer at various points in the diffusion field over the model can be used to provide estimates of pollutant concentrations in real (full scale) situations.

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*On assignment from the National Oceanic and Atmospheric Administration.

Figure 1. EPA meteorological wind tunnel.

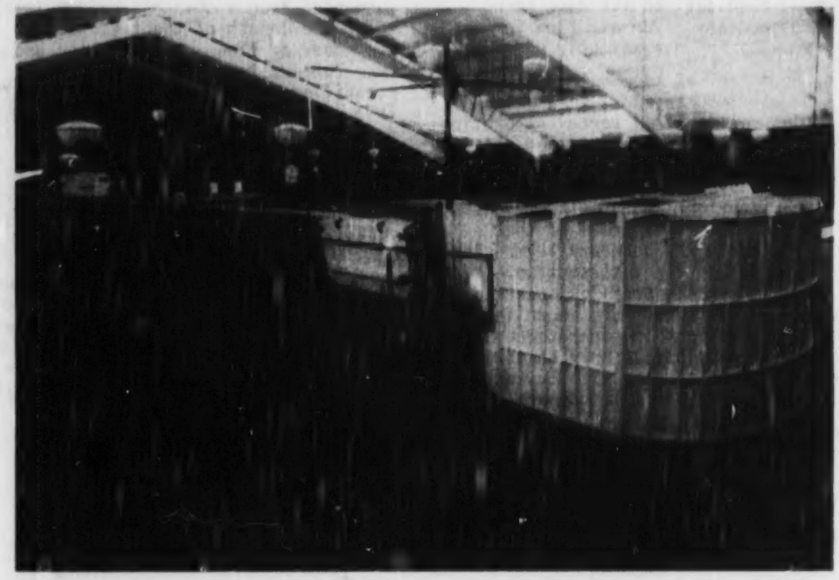


Figure 2. EPA water channel-towing tank.

Theoretical and Practical Considerations

Discussions of similarity considerations applicable to fluid modeling have been presented in the literature[2-4] and will not be repeated here. Compromises often must be made because all similarity criteria can not be satisfied simultaneously. It is evident that each laboratory has its own set of criteria, which may differ or even conflict with those of another laboratory. Also, other aspects of modeling, such as the minimum Reynolds number limit for similarity of plume rise, have not been completely established. A primary goal of the FMF, therefore, is to test the limits, determine the proper similarity criteria, and set the standards for fluid modeling of atmospheric dispersion.

Both air and water are suitable fluids to use as media for modeling atmospheric dispersion[2]. In principle, a factor of 15 in the Reynolds number may be gained by modeling with water as the medium. However, because of structural and pumping requirements, water facilities are normally much smaller and run at much lower speeds than wind tunnels. Thus, the full potential for obtaining larger Reynolds numbers using water flows is seldom realized.

Water has some advantages over air as the modeling medium. Flow visualization - using different colors of dyes, hydrogen bubbles, and neutrally buoyant particles - is generally much easier in water. Salts, acids, and dyes are used as tracers to determine pollutant concentrations when modeling dispersion characteristics in water. Water is also rather easily stratified using salt water layers of varying density; whereas, stratification in a wind tunnel requires rather elaborate heating and cooling systems.

Wind tunnels, however, have been used in many applications to simulate atmospheric motions. Flow visualization, velocity measurement, and concentration detection techniques have been developed and advanced to a level of high reliability and accuracy. Models used in wind tunnels need not be as solidly constructed or as firmly supported as those for use in water channels, where pressure forces are generally much larger. In addition, connections to probes do not require as much care with electrical insulation in air as in water, and there is less corrosion of metal.

Because both a wind tunnel and water channel-towing tank are available at the FMF, EPA scientists can use the one most suited to a particular research project.

Meteorological Wind Tunnel

The meteorological wind tunnel is an open-circuit, low-speed wind tunnel designed for simulating neutral atmospheric flows. The test section - 18 meters (m) long, 3.7 m wide, and 2.0 m high - has an adjustable ceiling to compensate for blockage when large models are used. Five subsections with interchangeable windows and floor units comprise the test section. A removable, 3.4 m diameter turntable can be placed in any of the five sections. The portion of a model installed on the turntable can be easily rotated to change the effective wind direction.

A 75 kilowatt (kW) a.c. motor driving a 1.8 m diameter fan through a speed controller (eddy current coupler) produces a top air speed of 10 meters per second (m/sec.). A carefully designed entrance-contraction section contains a honeycomb and four screens to produce a low turbulence flow at the entrance to the test section. The fan is downstream of the test section and is housed within a sound-deadening enclosure. Acoustic silencers in the flow both upstream and downstream of the fan provide for quiet operation.

An instrument carriage mounted on rails can position a probe anywhere in the test section. Controls to move the carriage in three dimensions are located on an operator's console near the tunnel. Digital readout indicates the position of the probe to the nearest millimeter.

Many methods have been devised for developing simulated atmospheric boundary layer air flow in wind tunnel test sections. The FMF has slightly modified a method devised by Counihan[5] at the Central Electricity Research Laboratories, England, to create power law wind profiles. Elliptical vortex-generating fins are placed just downwind of a castellated barrier at the entrance to the test section (Figure 3). The fins initiate a boundary layer with a thickness equal to their height. Two-dimensional roughness elements are placed on the tunnel floor downstream of the vortex generators to maintain the boundary layer characteristics over the length of the test section. Mean velocity and turbulence intensity profiles occurring 4 1/2 heights downwind of 1.8 m fins are shown in Figure 4. The mean velocity profile generated by this fin/roughness combination is close to a 1/5th power law, which is typical of flat country with low shrubbery. The turbulence intensity profile compares favorably with atmospheric data reported by Harris[6], which are shown in the figure for comparison. The FMF has 5 sets of these fins ranging from 15 to 180 centimeters (cm) in height. The fins may be easily inserted in the wind tunnel to obtain a boundary layer appropriate to the scale and characteristics of the model under test.

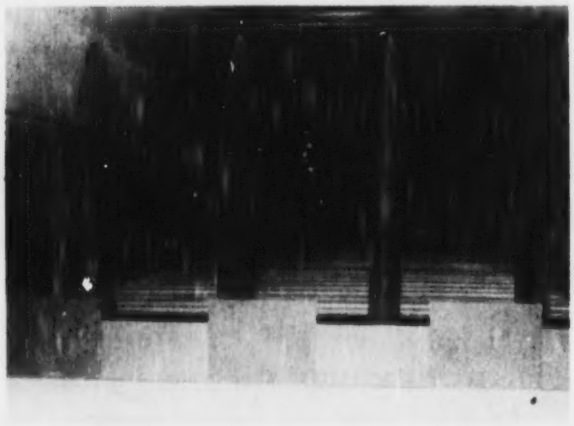


Figure 3. Elliptical vortex generating fins for developing simulated atmospheric boundary layers in meteorological wind tunnel test section.

Water Channel-Towing Tank

The water channel-towing tank was added to the FMF to make possible the study of dispersion under stably-stratified atmospheric conditions. As the name implies, it is a dual-purpose facility. Figure 2 shows its closed-circuit design, with the pump in the return leg on the bottom and the test section (free surface) on the top. The test section - 2.4 m wide, 1.2 m deep, and 25 m long - is constructed with floor and sidewalls of acrylic plastic in an aluminum framework.

In the towing tank mode of operation, the ends of the test section are blocked with gates and the test section is filled layer by layer with salt water, each layer of different density. Atmospheric temperature gradients are modeled by the density gradients of the salt water. Models are affixed to a turntable, suspended from a towing carriage into the fluid, and towed the length of the test section, making possible the study of flow and dispersion around buildings and over complex terrain and urban areas, under stably-stratified atmospheric conditions. The carriage speed is continuously variable from 0 to 0.5 m/sec. A filling system, consisting of a brinemaker and five large tanks, provides the capability of filling the test section with a desired stably-stratified salt-water mixture in approximately 4 hours.

In the water channel mode of operation, the facility is used in a manner similar to the wind tunnel procedure, with models fastened to the floor of the test section. A 1.5 m diameter pump, driven by a 75 kW a.c. motor through a speed controller (eddy current coupler), produces a top speed of 1.0 m/sec. The channel is supported on jacks that can be adjusted to tilt the entire unit to compensate for the pressure drop through the test section.

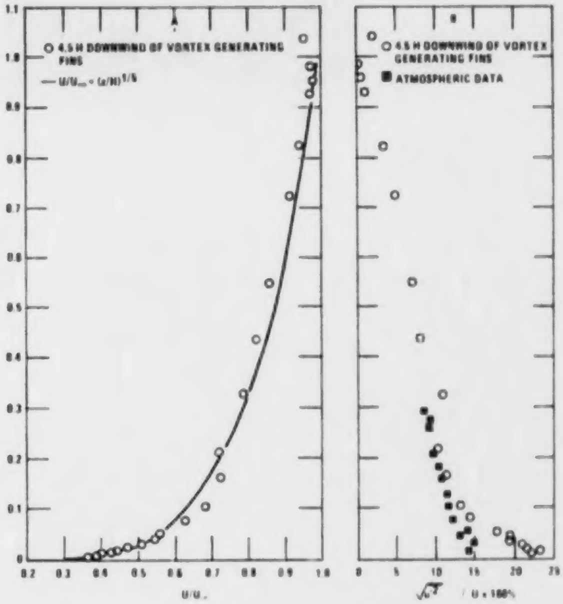


Figure 4. Vertical profiles of mean velocity (A) and local turbulence intensity (B) downwind of vortex generating fins (H=fin height=1.83m). Atmospheric data[6] are included for comparison.

Instrumentation

The FMF has a Digital Equipment Corporation PDP 11/40 minicomputer located within the facility to process all laboratory data. The system includes 3 magnetic tape drives, 3 disk drives, an 80K memory bank, a 16-channel analog-to-digital converter, a refresh-graphics terminal, and an electrostatic printer/plotter. It operates under RSX-11D, which is a multi-task, multi-user operating system. Real-time analysis of the outputs of electronic data gathering instruments provides instant feedback to the experimenter on the results of data being taken. The magnetic tape drives provide for economical storage of digitized data for future analysis.

Velocity measurements in the wind tunnel and water channel-towing tank are made with Thermo-Systems Inc. constant temperature hot-film anemometers. The outputs of the anemometers are digitized, linearized, and analyzed on the computer according to previously determined calibrations for each hot-film probe. Mean velocity and turbulence intensity values are printed out immediately after the last sample has been digitized for the scrutiny of the technician. Fast Fourier Transform techniques are used to obtain spectra and correlations of turbulence from signals recorded on magnetic tape. Programs have been written to calculate Reynolds stresses and velocity fluctuations in two coordinate directions from the output of cross-film probes.

In the wind tunnel, pollutant dispersion is studied by releasing a dilute tracer-gas-in-air mixture from the model source, collecting samples through a sampling tube, and measuring the concentration of tracer in the sample. Two Beckman model 400 Hydrocarbon Analyzers (flame ionization detectors) are used to determine the concentration of tracer in the sample. The output of the analyzer is also processed by the minicomputer. The response time of this system is too long to obtain statistics on concentration fluctuations, however.

Qualitative evaluations of dispersion patterns are made using flow visualization techniques. An oil fog generator produces a paraffin oil mist that is released from model sources in the wind tunnel; organic dyes are released in the water channel. By observing plume behavior and touchdown points, sampling locations for tracer measurements are determined. Still and motion picture cameras are used to photograph the experiments for a permanent record.

A metal and woodworking shop located within the FMF contains equipment and tools for constructing detailed models from metal, wood, and plastics. Minor modifications and additions to the facility are also performed in-house.

The FMF also houses an electronics shop for the repair and maintenance of instruments and other electronic equipment and for the development of new instrumentation.

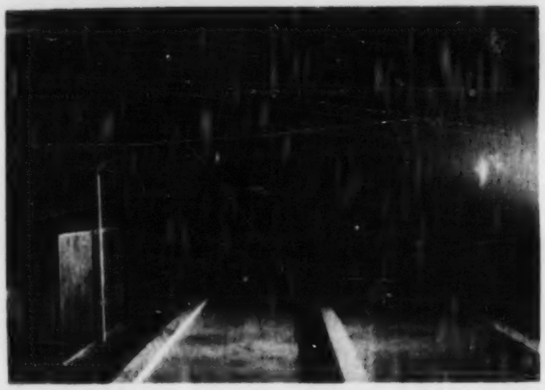
Applications

Because the water channel-towing tank has only recently been installed, specific applications are in the planning stages. Basic characteristics of the system are being studied, and modeling and measurement techniques are being developed for use in future projects. Some applications of the meteorological wind tunnel will be discussed.

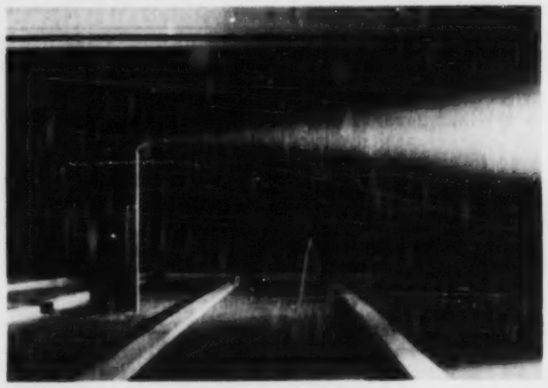
The first study completed in the meteorological wind tunnel was an analysis of the flow behind a two-dimensional mountain ridge to determine "rules of thumb" for the placement of smoke stacks. A cavity of recirculating flow was found in the lee of the ridge with a height equal to approximately twice the ridge height and a length equal to ten ridge heights. A summary paper[7] on this work will be presented at this conference.

Wind tunnels are often used to evaluate aerodynamic influences of buildings on smokestack plumes. Unique characteristics of specific emission sites or building shapes may require exact modeling of individual cases. The FMF is more involved with the analysis of general cases from which general conclusions or "rules of thumb" can be obtained.

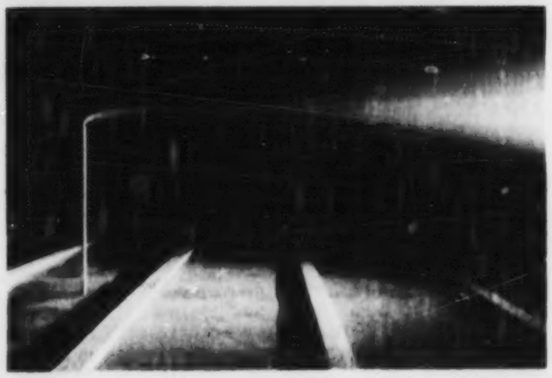
One such study[8] was performed to test the notion that a stack must be 2 1/2 times as high as the tallest nearby building to avoid plume downwash resulting from building effects. Two buildings were used; one with its width twice its height and one with its width one-third its height. The 2 1/2 times rule was found to be unnecessarily conservative for the thin building. Smoke visualization photographs are presented in Figure 5 for a stack that is 1.5 times the



5(a) building width twice its height



5(b) building width 1/3rd its height



5(c) stack without building

Figure 5. Plume visualization for a stack 1 1/2 times as high as nearby building. Building heights, stack heights, and boundary layer and effluent characteristics are identical in all three photographs.

building height for the wide building, the thin building, and no building. Comparison of the photographs shows that, even though the stack heights and building heights are identical, the wide building produces strong plume downwash, whereas the thin building has essentially no influence on the plume. Quantitative concentration measurements verified the visualization results.

The influence of buildings on stack emissions was more thoroughly investigated in a cooperative study[9] performed in response to a request by the EPA Office of Air Quality Planning and Standards (see Figure 6). One building with width equal to twice its height, H_B, was used. The stack was located at the center of the downwind side of the building. Emphasis was placed on quantifying the building influence on ground level concentrations as a function of stack height, H_S, stack diameter, D, exit velocity, W, and buoyancy. Many combinations of these parameters were examined both with and without the building in place. Figure 6 presents ground level concentrations measured under the plume centerline for a stack that is 1 1/2 times as high as the building. Measured concentrations for a ground release in the building wake are also presented. A mathematical model based upon a Gaussian plume formulation with a correction for increased dispersion behind the building has been found to approximate the data reasonably well.

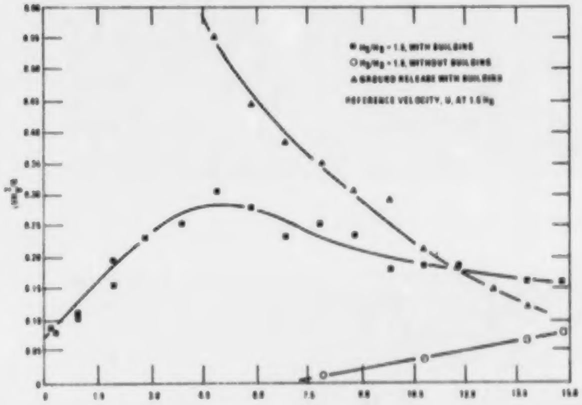


Figure 6. Nondimensionalized ground level concentration for neutrally buoyant plume. D/H_B = 0.063, W/U = 0.7.

Another model constructed for study in the meteorological wind tunnel involved moving 1:32-scale-model vehicles to simulate highway traffic (Figure 7). The vehicles are pulled across the test section by a chain imbedded in the floor of the turntable. Characteristics of the turbulent wake region downwind of moving vehicles are to be determined. Preliminary results show that the vehicle-induced mechanical turbulence has a strong influence on the dispersion of vehicle exhaust close to the highway.

Through studies of this type, a general understanding of the mechanisms of atmospheric dispersion can be gained. EPA Fluid Modeling Facility scientists intend to concentrate efforts on this type of project as opposed to evaluating specific case studies involving circumstance peculiar to a given topographical location or building design. In conjunction with these studies, modeling techniques and similarity theories will be evaluated to establish guidelines for proper modeling methods.

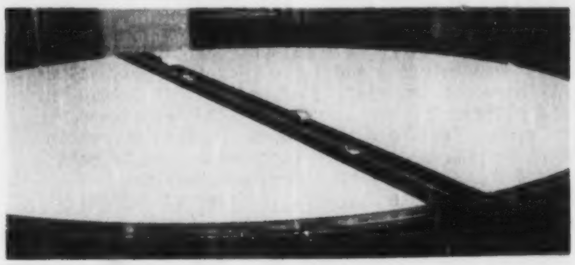


Figure 7. Highway model with moving vehicles on meteorological wind tunnel turntable.

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PLUME BEHAVIOR IN THE LEE OF A MOUNTAIN RIDGE -- A WIND TUNNEL STUDY

Alan H. Huber
Monitoring and Data Analysis Division
Office of Air Quality Planning and Standards

William H. Snyder*
Roger S. Thompson
Meteorology and Assessment Division
Environmental Sciences Research Laboratory

and

Robert E. Lawson, Jr.
Northrop Services, Inc.

Work Performed In
Fluid Modeling Facility
Meteorology and Assessment Division
U.S. Environmental Protection Agency
Research Triangle Park, N. C. 27711

Summary

A wind tunnel study of the concentration field resulting from a stack placed in the highly turbulent region downwind of a two-dimensional mountain ridge is presented. This highly turbulent region, often referred to as the "cavity," was found to consist of a large semipermanent eddy. The general circulation was in the main flow direction along the upper edge, opposite the main flow direction along the ground surface, and up the slope along the leeward ridge surface. The eddy is a result of the main flow separating at the apex of the ridge. A stack was positioned to emit an air-methane mixture into the cavity in the lee of the ridge. Longitudinal, lateral, and vertical concentration profiles showed that a tall stack placed near the upper boundary of the cavity resulted in higher ground level concentrations near the downwind end of the cavity than did a short stack. The highest ground level concentrations, however, were found to occur near the base of the short stack. Application of the "2.5 times rule" with respect to the ridge height was found to be sufficient for avoidance of the highly turbulent region.

Introduction

Background

Aerodynamic effects induced by local terrain features can have a major influence upon the dispersion of locally emitted effluents. Even with the best demonstrated control technology applied, most plume concentrations at the stack exit are at levels far in excess of ambient air quality standards. The plume may frequently be entrained in the turbulent eddies created by air flow over local terrain features and be brought to the ground before the concentrations are sufficiently reduced to levels below ambient air quality standards. These effects are often referred to as "plume downwashing."

This paper discusses the results of a set of experiments designed to examine the highly turbulent region that can be found on the leeward side of a steeply sloping mountain ridge. The study was conducted in the meteorological wind tunnel at the Fluid Modeling Facility of the U. S. Environmental Protection Agency (EPA). Fluid modeling is ideally suited for investigations of the complex plume behaviors that result from aerodynamic effects because essential variables can be controlled and examined at will.

For neutral (neutrally stable) atmospheric flows, aerodynamic effects evolve from interacting frictional forces and pressure gradients induced by local surface roughness and terrain features. Adverse effects exist when surface friction and pressure gradients combine to retard the surface layer flow enough to produce separation of the boundary layer. Separation in a neutral flow generally occurs near the apex of the terrain feature resulting in development of a stagnation region on the leeward side, often referred to as a "cavity." At the point of separation, the main stream of flow is vertically raised, resulting in the development of a stagnation region (cavity) below, where mean velocities are reduced and the flow is highly turbulent. The flow reattaches itself somewhere downstream of the obstacle. In the region of reattachment, a portion of the flow is deflected upstream, forming a zone of recirculation. The dividing "streamline" that separates the recirculating flow from the main stream encloses the cavity, as shown in Figure 1. The "wake region," which is defined as that region of the flow field that is disturbed by the obstacle, can extend far downwind. The "envelope" is the upper boundary of the wake region. Far enough downwind, of course, the flow readjusts itself to a boundary layer appropriate to local surface roughness.

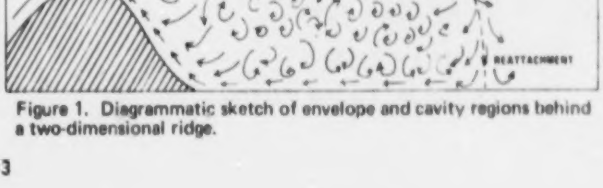

Figure 1. Diagrammatic sketch of envelope and cavity regions behind a two-dimensional ridge.

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* On assignment from the National Oceanic and Atmospheric Administration.

Literature Review

A review of published field studies,[1-11] supports the assertion that, on the leeward side of a mountain ridge, a recirculating flow region with strong downwash and enhanced dispersion exists. Consistent information that could define the point of separation and the size and extent of the cavity was not found, however. The point of separation appears to be very much a function of mean flow speed and direction, atmospheric stability, both the downslope and upslope angle of the ridge sides, and the location of the ridge with respect to surrounding terrain.

For a particular situation, the cavity will be largest when separation occurs at the ridge apex. Obstructions with sharp edges should exhibit definite separation at those edges under all atmospheric conditions. The size of the cavity region is greatest for isolated ridges with steep sloping sides. Stable atmospheric conditions act to restrict the size and extent of the cavity region.

Experimental Plan

Terrain features that most adversely affect the flow are two-dimensional in nature. Lateral air motion around a hill results in a smaller cavity size than would be observed for a two-dimensional ridge. A study of neutral flow with separation occurring at the apex of a two-dimensional mountain ridge best demonstrates the extent to which stagnation regions can influence the dispersion of locally emitted effluents.

There were three major phases to this study. Phase I involved a Gaussian ridge and a triangular ridge. Velocity and cavity size measurements were made in order to demonstrate that the basic flow structure is independent of the detailed shape of the ridge. Phase II involved mapping of the concentration field resulting from a source placed within the cavity. Phase III examined the effect of variations in the approach flow on the cavity size and shape. This presentation emphasizes the results of the second phase. The complete description of these studies is given in Huber, et al.[12]

Experimental Details

Similarity Criteria

In order to ensure that the flow in the model simulates that in the atmosphere, it is necessary to meet certain similarity criteria. Various nondimensional parameters characterizing the flow in the atmosphere must be matched in the model. Because this study is concerned only with neutral atmospheric flows, non buoyant effluents, and relatively small scales, the Richardson, Froude and Rossby numbers may be ignored (Snyder[13]). The remaining parameters of significance are as follows:

$$\frac{L}{H}, \frac{H_s}{H}, \frac{D_s}{H}, \frac{\delta}{H}, \frac{U}{U_\infty}, \frac{\left(\overline{u'^2}\right)^{1/2}}{U}, \frac{W_s}{U_s}, \frac{U_\infty H}{\nu}, \text{ and } \frac{W_s D_s}{\nu},$$

Where: L = characteristic width of ridge

H = height of ridge

H_s = height of stack

D_s = inside diameter of stack

δ = boundary layer thickness

U = mean wind speed (a function of elevation)

$\left(\overline{u'^2}\right)^{1/2}$ = root-mean-square of longitudinal velocity fluctuations

W_s = stack effluent speed

U_s = wind speed at top of stack

ν = kinematic viscosity of air

The first four of these parameters (length ratios) are easily matched by constructing a scale model, but because no particular field situation was modeled, idealized ridge shapes and representative values were chosen. The fifth and sixth parameters characterize the boundary layer approaching the ridge. Two different boundary layers were used. A vortex generator-roughness element combination similar to that of Counihan[14] was used to provide a 60-cm atmosphere-like boundary layer. The other was the natural (δ=15-cm) boundary layer developed over the smooth wind tunnel floor.

The effluent speed to wind speed ratio was maintained at 3:2 in all tests. This value is the minimum necessary to avoid downwash in the immediate lee of the stack itself (Sherlock and Stalker[15]).

Plume rise or downwash from the model stack placed in the lee of the ridge are, therefore, associated with disturbances induced by the ridge. The diameter to ridge height ratio was kept at a value equal to 0.03 in reference to the 30 cm model ridge.

The last two parameters are the ridge Reynolds number ($Re_H = U_\infty H/\nu$) and the effluent Reynolds number ($Re_D = W_s D_s/\nu$). For exact similarity, the model ridge Reynolds number must equal the actual ridge Reynolds number. This was not possible for the model scales used and, fortunately, is not necessary (Snyder[13]) because the flow fields become independent at sufficiently large Reynolds number. For a mountain ridge with a salient edge near the peak, the boundary layer may be expected to separate at the edge (Scorer[2]). If the point of separation on the model occurs at its apex, similarity of the two flow patterns should result. The plume behavior should be independent of the effluent Reynolds number provided the flow is fully turbulent at the stack exit. Internally serrated washers were placed inside the stack to ensure fully turbulent flow at the exit.

Equipment

The wind tunnel test section measures 3.7 m x 2.1 m x 18.3 m. The flow speed within the wind tunnel can be controlled between 0.3 and 10 meters per second (m/sec). The ceiling of the wind tunnel can be adjusted to compensate for blockage effects of the models. In this study, the ceiling was adjusted to obtain a nonaccelerating free-stream flow above the mountain ridge. Further details of the wind tunnel may be obtained from Snyder, et al.[16]

Three model ridges were constructed. One ridge was triangular in shape with a 30.5 cm high apex and sloping sides of 30°; the other two had sides with idealized shapes. The ridges were symmetrical about a center line, each side of which could be divided into three sections. The center section had a constant slope of 30°. The upper and lower sections were respectively convex and concave outward. This model shape appears to be very close to a Gaussian probability distribution and is referred to as the Gaussian model ridge in order to distinguish it from the triangular model ridge.. The two similar Gaussian ridges had apexes of 30.5 cm and 15.2 cm, respectively. The three models will be referred to in the remainder of this report as the 30-cm triangular ridge, the 30-cm Gaussian ridge, and the 15-cm Gaussian ridge.

For mean velocity and turbulence intensity profiles, a Thermo-Systems Inc. Model 1054 A anemometer was used in conjunction with their Model 1210-20 hot-film probes. Smoke visualization studies made use of an oil-fog generator.

An air-methane mixture was ejected from the stack as a tracer gas. This effluent simulated a neutrally buoyant plume because the amount of methane in the gas mixture was only 1 percent and the stack gas temperature was equal to the ambient air temperature.

Concentration profiles were obtained by sampling a stream through a Beckman Model 400 Hydrocarbon Analyzer, which is a flame ionization detector. Its response time of 0.5 second is too long to examine any dispersion micro-structure. Time averages can be related to steady-state averages occurring in similar full scale situations, however. A 2.5 minute averaging time was found to yield stable values of concentration.

Experimental Concentrations

Concentrations measured in the model may be related to steady-state averages that would be measured in the field. The stack gas concentration, C_s, is related to the emission rate by

$$Q=C_s[(\pi/4)(D_s^2)]W_s. \qquad (1)$$

The field concentration, C_F, is linearly related to the model concentration, C_M, to the emission rates, Q_F, and to the dilution ratio, $U_M H^2_M/U_F H^2_F$. These basic relations result in the expression

$$C_F=(C_M)(Q_F/Q_M)(U_M/U_F)(H_M/H_F)^2\text{, or} \qquad (2)$$

$$(C/C_s)_F=(C/C_s)_M[(W_s/U_s)_F/(W_s/U_s)_M][(D_s/H)^2_F/(D_s/H)^2_M].$$

With identical effluent speed to wind speed ratios and stack diameter to ridge height ratios, the model concentration ratios are equal to the field concentration ratios,

$$(C/C_s)_M = (C/C_s)_F. \qquad (3)$$

Experimental Results

Phase I

Smoke Visualization. For flow separation to occur at the apex of the 30.5-cm Gaussian ridge, a tripping device was required. A small square rod was placed along the ridge apex to induce flow separation. With flow separation at the apex, the cavity depth and length were two times larger than for the cases without and were independent of the mean flow speed. Flow visualization measurements behind the 30-cm triangular ridge resulted in similar size and shape of both the cavity and envelope as those for the tripped 30-cm Gaussian ridge (Figure 2).

Mean Velocity and Turbulence Intensity.

The mean velocity and turbulence intensity profiles for both upstream and downstream positions from the tripped 30-cm Gaussian ridge are presented in Figure 3. The 60-cm atmosphere-like boundary layer was used as the approach flow. The mean velocity, U, is defined as the 1-minute average flow speed in the longitudinal direction, x. The turbulence intensity is defined as the standard deviation of the velocity fluctuation in the longitudinal direction, normalized with the local mean velocity. Measurements in regions having mean flow reversals are not quantitatively valid because the hot-film cannot distinguish flow direction. Smoke visualization quite clearly revealed upstream flow near the surface level. The data presented, however, should permit valid qualitative comparisons.

The degree of disruption of the approach flow was found to be small in extent for the untripped ridge. The profiles around the 30-cm triangular ridge were found to compare quite well with those of the tripped 30-cm Gaussian ridge. For those cases in which flow separation occurred at the apex of the model, the profiles were found to be independent of the free-stream velocity.

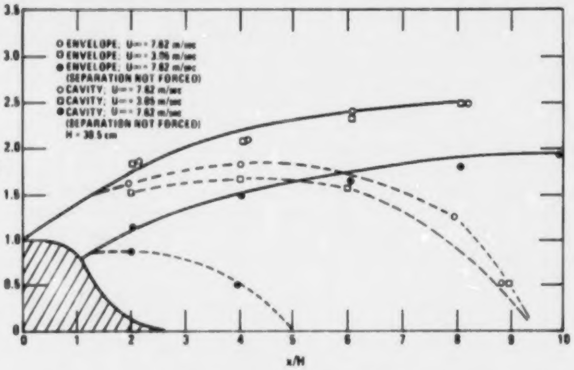

Figure 2. Cavity and envelope size in lee of 30.5-cm Gaussian ridge.

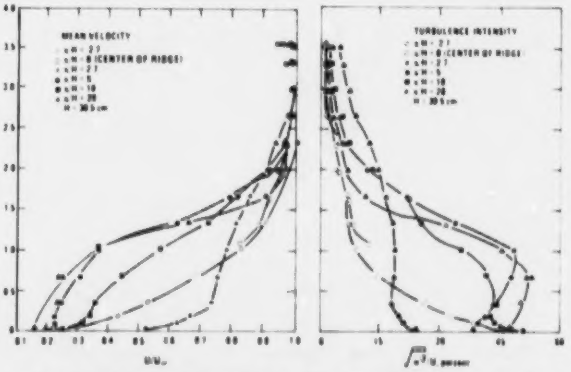

Figure 3. Mean velocity and turbulence intensity profiles for the 30.5-cm, tripped Gaussian ridge, U∞ = 3.05 m/s.

Phase II

Concentration measurements are presented in the figures in order to assist in describing plume behavior within the cavity region in the lee of the 30-cm tripped Gaussian ridge. To present the data in a form for easy comparison, the measured concentrations have been nondimensionalized with the stack gas concentration, C_s. Thus, the value "C, percent" in the figures is the measured concentration expressed as the percentage of stack gas concentration. This value can be directly related to average field concentrations as discussed earlier. A field situation with the stack emission concentration equal to 2000 ppm would result in the air quality measurement of 1 ppm under circumstances similar to those of the model where C percent is equal to 0.05.

Concentration Measurements. The concentration values in Figure 4 were detected by a ground level probe located near the base of the 30-cm tripped Gaussian ridge. The stack was positioned at four different downwind locations and raised to various heights while the probe sampled at the fixed position. The stack height where no ground concentrations were detected defined the limit of the cavity. The fact that significant ground level concentrations are found at a distance of 5 H upwind of the stack demonstrates the existence of a strong recirculating flow within the cavity region. The size of the cavity determined from the tracer gas measurements (Figure 4) showed a maximum depth and horizontal extent of 2 H and 8.5 H, respectively. The horizontal extent was only slightly smaller than that found by smoke visualization (10 H) for the same situation (Figure 2).

Figure 5 gives the resulting ground level concentrations downwind from a stack placed at the leeward base of the tripped ridge for three stack heights. Maximum concentrations are found very close to the stack base. The peak concentration decreases and is shifted downwind as the stack height increases. This pattern is typically found to occur over flat terrain. Beyond two ridge heights downwind from the stack, however, the concentrations are highest for the tallest stack, which is not at all typical of plume behavior over flat terrain.

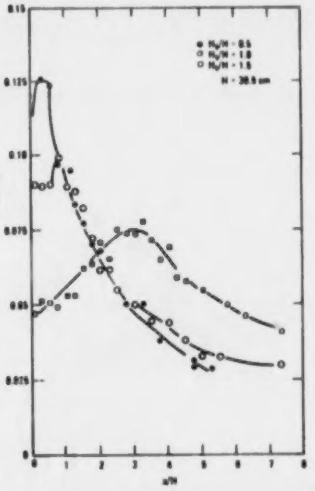

Figure 5. Longitudinal ground level concentration profiles downwind from stack placed at base (x/H = 2.7 from center) of 30.5-cm tripped Gaussian ridge.

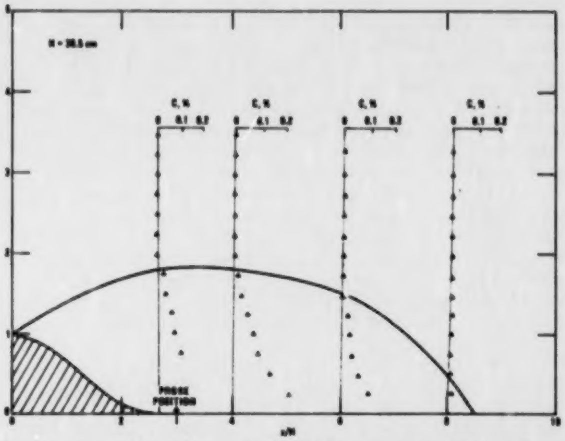

Figure 4. Ground level concentrations measurements with sampling probe fixed near base (x/H = 3 from ridge center, z/H = O) of 30.5-cm, tripped Gaussian ridge (stack was placed at four downwind locations and its height was varied).

Figure 6a presents some vertical concentration profiles in the lee of the tripped ridge. The stack was fixed at the ridge base with the height of the stack measuring one-half the ridge height. Because of nearly stagnant mean flow in the lee of the ridge and the general upward flow in the cavity region along the ridge surface, a substantial plume rise occurs -- as is indicated by the vertical concentration profiles. The concentrations on the leeward side of the cavity are more uniform than those farther upstream, but little spreading occurs into the region above the cavity (z/H>2). The lateral concentration profiles in Figure 7a show that the lateral plume width changes only slightly in the downwind direction..

Additional concentration measurements for the same stack and location, but with stack height 1.5 times the ridge height, were also made. Figure 6b presents a few vertical concentration profiles for the elevated stack and shows the plume rise to be essentially zero. Zero plume rise now occurs because the elevated stack is above the region of mean flow stagnation. The elevation of the point of maximum concentration decreases with downwind distance, showing evidence of the recirculation within the cavity. The highly uniform concentrations below z/H = 1 are also evidence of the recirculation. Even for this elevated stack, little dispersion into the region above the cavity occurs. The lateral ground level concentration profiles in Figure 7b show essentially identical spread with only minor differences in their values near the center (y/H = 0). From these results, it is evident that instead of the strong immediate downwash, which occurred for the shorter stack, the taller stack emissions are caught in the outer recirculation region within the cavity. The direction of the recirculation is down the leeward side of the cavity and upstream along the ground. Concentrations measured near the reattachment point were highest for the 1.5 H stack. This occurs because emissions near the upper boundary of the cavity region are caught in the general recirculation that downwashes the plume towards the reattachment point. Because emissions from a shorter stack at the same location as above are more rapidly downwashed and dispersed, a lower concentration will occur at the reattachment point. This is one instance in which increasing the stack height does not decrease ground level concentration.

Phase III

The goal was to determine the effect of the approach boundary layer conditions on the size and shape of the leeward cavity region. The cavity size and envelope for the 60-cm atmosphere-like boundary layer approaching the 15-cm Gaussian ridge were found to be similar to those for the 15-cm natural boundary layer. The turbulence levels of the approaching natural boundary layer may be expected to be much lower than those of the simulated atmospheric boundary layer.

Changes in the size of the cavity and the envelope were found when the mean flow approached the ridge along a plane elevated to the height of the ridge apex. Both the wake and envelope size were reduced in comparison with the cases for an isolated ridge. The effect of changing the boundary layer conditions appears to be minor in comparison with effects of upwind terrain changes.

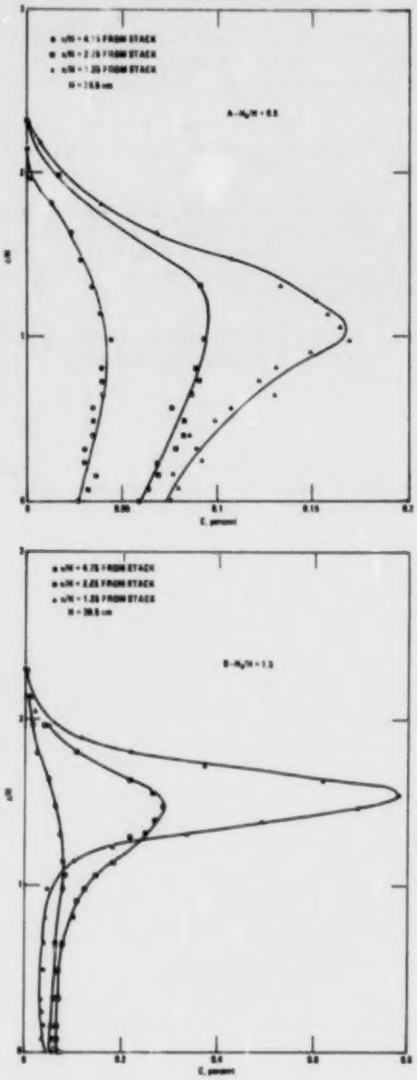

Figure 6. Vertical concentration profiles for stack placed at base (x/H = 2.7 from center) of 30.5-cm tripped Gaussian ridge. A - H_s/H = 0.5; B - H_s/H = 1.5.

Conclusions

For the 30 cm Gaussian ridge with separation occurring at the apex, the maximum depth and horizontal extent of the cavity region were found to be 2 H and 10 H, respectively. The flow patterns in the lee of ridges that exhibited separation at their apex were found not to be sensitive to the detailed shape of the slopes. The cavity sizes and shapes were found to be only slightly affected by the thickness and turbulence intensity of the approach boundary layer, but were dependent upon the upwind slope of the terrain.

Near the downwind end of the cavity (that is, near the reattachment point), the flow is difficult to characterize. Part of the main flow recirculates within the cavity, and the rest continues downwind forming a newly developing boundary layer. This region can best be characterized by the increased vertical and lateral spreading of a plume over that occurring for a flow without the mountain ridge disruption. The above assertions are generalizations drawn from a limited amount of smoke visualization and mean velocity and turbulence intensity data taken downwind of the reattachment point. Further studies of the behavior of plumes from stacks placed downwind of the reattachment point are needed to characterize dispersion there.

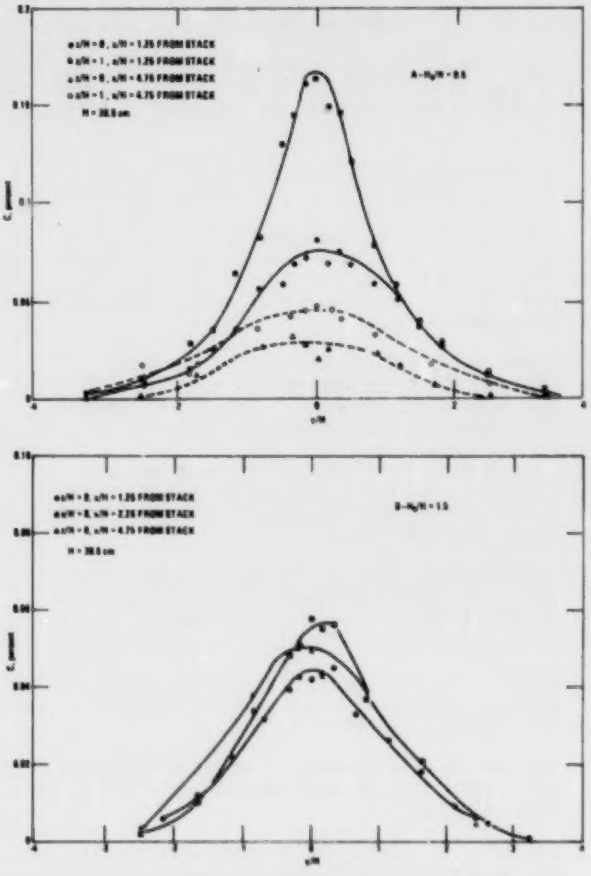

Figure 7. Lateral concentration profiles from stack placed at base (x/H = 2.7 from center) of 30.5-cm, tripped Gaussian ridge. A - H_s/H = 0.5; B - H_s/H = 1.5.

The cavity region leeward of the model ridge was found to be highly turbulent with significant plume downwash. The plume downwash results in ground level concentrations within the cavity region that are greater than 0.05 percent of the stack effluent concentration. These concentrations are undoubtedly significantly higher than would occur in the absence of the mountain lee effects examined in this study. For similar actual situations, it would be good engineering practice to avoid placement of any significant source within the expected cavity region.

The general engineering "rule of thumb," as found repeatedly throughout the literature, for avoiding plume downwash in the lee of an obstruction is to keep the height of the stack "2.5 times" the height of the obstruction. According to Sutton,[17] the rule was probably derived by Sir David Brunt from a study on the height of disturbances over a long ridge in connection with a British airship disaster investigation. It, therefore, is not surprising that the general rule is applicable to the results of this study. Although the maximum depth of the cavity was found to be 2 H, some margin of safety is well advised, because strong downwashing occurs in the upper regions of the cavity. The maximum horizontal extent of the cavity was found to be 10 H. Part of a plume emitted above a cavity can, in this distance, spread downward and thus become entrained within the cavity.

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A NOTE ON THE SEA BREEZE REGIME

S. Trivikrama Rao
Division of Air Resources
New York State Department of Environmental Conservation
Albany, New York

Perry J. Samson
Department of Meteorology
University of Wisconsin
Madison, Wisconsin

ABSTRACT

Rotary spectrum analysis is applied to the wind field over Long Island, New York, to delineate the clockwise and counterclockwise turning associated with various spectral frequencies. On the south shore and at higher elevations elsewhere over the island, the diurnal oscillation is found to be a predominantly clockwise rotation derived from sea breeze. At lower levels, mid-island and on the north shore, there is no dominant rotation in the diurnal oscillation. This may be attributed to the interaction between the sound breeze from Long Island Sound and the sea breeze from the Atlantic Ocean.

INTRODUCTION

The sea breeze regime is mainly driven by the difference between the air temperature over land and that over water. The diurnal variation of solar radiation sets up a temperature contrast between the two surfaces because of their different heat capacities. Because of the influence of the Coriolis acceleration, the rotation of the sea breeze is predominantly clockwise.

The Long Island Sound to the north and the Atlantic Ocean to the south of Long Island produce sound breezes and sea breezes, respectively, resulting in complex circulation patterns over the island. Rotary spectrum analysis provides a means of distinguishing the presence of clockwise and counterclockwise rotation components in the horizontal wind field and is an excellent tool to study such interactions.

This paper reports the results of rotary spectrum analysis of the wind data collected on the north and south shores and in the center of Long Island, New York.

SOURCE OF DATA

Data from wind direction and speed sensors were obtained from towers located on the south shore of Long Island at Tiana Beach, on the north shore at Shoreham and Jamesport, and in the center at Brookhaven National Laboratory (BNL). These locations are shown in Fig. 1. Hourly values were collected from sensors at 75 ft. at Tiana Beach, 355 ft. at BNL, 33 ft. and 150 ft. at the Shoreham tower and 400 ft. at Jamesport tower. Data for the period July-August 1975, representative of summer, are used in this study. Data for December 1974-January 1975 at 355 ft. level at BNL, representative of winter, are also analyzed to explore the seasonal variation of the different spectral components.

METHOD OF ANALYSIS

Gonnella[1] used the rotary spectrum to study internal waves in the ocean. This type of analysis has since been applied to the study of the sea breeze regime along the coast of Oregon by O'Brien and Pillsbury[2]. Basically, the method hinges on the fact that the spectral decomposition gives at each frequency (f) a sinusoidal wave for each horizontal velocity component. The east and north component sinusoids together form an ellipse at each frequency. Four quantities emerge in the rotary spectrum analysis: the mean kinetic energy or the total spectrum, the rotary coefficient, and the orientation and stability of the ellipse. All these quantities, except the orientation of the ellipse, are invariant under coordinate rotation. If P_{uu}, P_{vv} are the auto-spectra and P_{uv}, Q_{uv} are the cross and quadrature spectra of the east and north components, u(t) and v(t), of the horizontal velocity, the following mathematical relationships exist:

The total spectrum:

$$S_f = C_f + A_f = 1/4\ (P_{uu} + P_{vv})$$

where the clockwise spectrum:

$$C_f = 1/8\ (P_{uu} + P_{vv} - 2\ Q_{uv})$$

and the anti clockwise spectrum:

$$A_f = 1/8\ (P_{uu} + P_{vv} + 2\ Q_{uv})$$

The rotary coefficient:

$$C_R = \frac{C_f - A_f}{S_f} = \frac{-2\ Q_{uv}}{P_{uu} + P_{vv}}$$

The orientation of the ellipse:

$$\tan 2\ \phi = \frac{2\ P_{uv}}{P_{uu} - P_{vv}}$$

and the stability of the ellipse:

$$|E|^2 = \frac{(P_{uu} + P_{vv})^2 - 4\ (P_{uu}\ P_{vv} - P^2_{uv})}{(P_{uu} + P_{vv})^2 - 4\ Q^2_{uv}}$$

The rotary coefficient, C_R, varies as $(1 - \epsilon)$ where ϵ is the eccentricity of the ellipse. Its numerical value ranges from 0, indicating unidirectional motion, to unity, a pure rotary motion. Further descriptions of the spectrum may be found in Gonnella[1].

For the statistical analysis presented here, a fast Fourier transform algorithm is used to partition the sample variance among frequency bands. The total length of the data is divided into 5 non-overlapping segments each consisting of 256 data points (N = 256), so that the spectral estimates have 10 degrees of freedom. This technique is discussed by Hinich and Clay[3]. To avoid end effects, the N points are smoothed by use of a weighting function of the form $1/2\ (1 - \cos \frac{2\pi n}{N})$, n = 1, 2....N. In addition, the trend is removed by subtracting a linear function from the data values. These data are Fourier-transformed to derive the complex Fourier coefficients from which the clockwise and anticlockwise spectra are computed for each segment, and then averaged over all segments. Furthermore, these spectral estimates are subjected to a "Double-Hanning" smoothing procedure (Jenkins and Watts[4]) which increases the reliability of the spectral estimates.

RESULTS

The variance spectra for the wind field at Tiana Beach, Fig. 2a, shows the dominance of the clockwise rotation at the diurnal and semi-diurnal frequencies. The spectra at BNL and Jamesport, Fig. 2b and 2d respectively, do not reveal any anticlockwise rotation at the diurnal frequency. The peak corresponding to f = 0.04 cycles/hr at these elevated sensors is predominantly a clockwise rotating oscillation, a sea-breeze phenomenon. The spectra at the 33 ft. level at Shoreham (Fig. 2e) show no clear dominance of rotation. However, at the 150 ft. level (Fig. 2f) the dominance of clockwise rotation is again seen. Also included is the spectrum for winter season at BNL 355 ft. level (Fig. 2c). Note the complete absence of diurnal and semi-diurnal peaks suggesting that the influence of the large-scale weather features, dominant in the winter season, overshadows the sea-breeze circulation generated by the land and water temperature difference

The rotary spectral statistics are presented in Table 1. The lower bound on values of the ellipse stability at the 1% confidence level is 0.63 (Panofsky and Brier[6]). This implies that the chances are 1 in 100 that a stability coefficient of 0.63 or more will be found by accident. It is evident from the table that the ellipse stabilities at Shoreham 150 ft., Tiana Beach 75 ft., BNL (summer) 355 ft., and Jamesport 400 ft. exceed this limiting value. Also, C_R values of 0.73 at the BNL (summer) and 0.66 at Jamesport indicate a strong rotary motion at the upper levels. At the Shoreham 33 ft. level a C_R value close to zero and insignificant ellipse stability coefficient imply no dominance of any particular direction in the oscillation. At the upper levels, an average value of the orientation of the major axis of the ellipse is found to be 76° (from true north) which corresponds to the orientation of the Long Island coastline. This indicates that on eastern Long Island, local circulation patterns are generally aligned in axes parallel to the shoreline.

TABLE 1

Rotary Spectral Statistics for the Diurnal Oscillation

Station	Height of Observation(ft)	Orientation of the ellipse(ϕ)	Rotary Coefficient (C_R)	Ellipse Stability(E)	$\frac{C_f}{A_f}$
Shoreham	33	275°	0.07	0.31	1.25
Shoreham	150	83°	0.32	0.88	1.81
Jamesport	400	70°	0.66	0.77	3.88
BNL(Summer)	355	75°	0.73	0.72	4.77
Tiana Beach	75	78°	0.42	0.80	2.45
BNL(Winter)	355	347°	0.24	0.20	1.68

The effect of friction on the sea breeze hodograph tends to render the ellipse smaller and considerably more eccentric. Large eccentricity values for the diurnal oscillation found at lower levels can be attributed to the influence of friction at the lower boundary. It should be recalled that the rotary coefficient values vary as $(1-\epsilon)$ where ϵ is the eccentricity. The decreasing values of eccentricity (increasing C_R) with height reflect the decrease in frictional influence. The eccentricity found at Tiana Beach is less than that at the Shoreham 150 ft. level. This may be explained by the interaction of sound breeze and sea breeze on the north shore.

Haurwitz[7] described the relationship between the maximum temperature difference between land and water as a function of coefficient of friction. He suggested that without friction the time difference between maximum sea-breaze velocity and maximum land and water temperature contrast is 6 hours. With increasing friction, the time difference between the maximum of the sea breeze velocity and that of temperature difference decreases. The average shape of the diurnal wave can be obtained through superposition of several diurnal cycles in the record, and then averaging the specific value for each phase of the wave. When this is done, it is found that the wind speed maximum occurs around 17:00-18:00 EST at Tiana Beach and at the Shoreham 33 ft. level; and around 20:00 EST at Shoreham 150ft., BNL 355 ft., and Jamesport 400 ft. levels. With such values of friction as have been determined from observations on land, the maximum sea breeze should occur about three hours after the temperature difference between land and water has reached a maximum. Usually, the maximum temperature difference occurs about 14:00-15:00 EST. The decrease of frictional effects with height could explain the larger time difference between maximum wind speed at Shoreham 150 ft., BNL 355 ft., and Jamesport 400 ft. levels and maximum land and water temperature difference, consistent with the rotary coefficient values.

A study of the characteristics of the Atlantic sea breeze and Long Island sound breeze (LILCO[8]) concluded that the sound breezes are generally morning phenomena and have onset times between 09:00 EST and 12:00 EST. The average duration of the sound breezes was about three hours after which they were generally destroyed by the strengthening of the Atlantic sea breeze. They also found that the stronger Atlantic sea breeze is capable of overrunning the sound breeze completely, resulting in a flow reversal from on-shore to off-shore near Shoreham. Dominance of clockwise rotating oscillation in the rotary spectra at upper levels lends support to their observation. The dynamics of the interaction of the sea and sound breezes at Shoreham probably account for the lack of an easily discernable rotation pattern.

SUMMARY AND CONCLUSIONS

A relatively new descriptive technique to analyze vector time series, the so-called rotary spectrum, has been applied to study the sea-breeze circulation over eastern Long Island, New York. The results indicate a clear dominance of the sea breeze at levels above 150 ft. The hodographs show a pronounced eccentricity at lower levels, a manifestation of friction. The observed phase differences between occurence of maximum wind speed over land and maximum land and water temperature difference are consistent with the sea-breeze dynamic theories. Furthermore, as to be expected, during the winter season the local sea-breeze pattern set up by the land and water temperature contrast has been completely overshadowed by large-scale weather features. In future studies, it would be interesting to compute the trajectories of the wind field over Long Island to obtain more quantitative information on the nature of sound and sea breezes.

ACKNOWLEDGEMENTS

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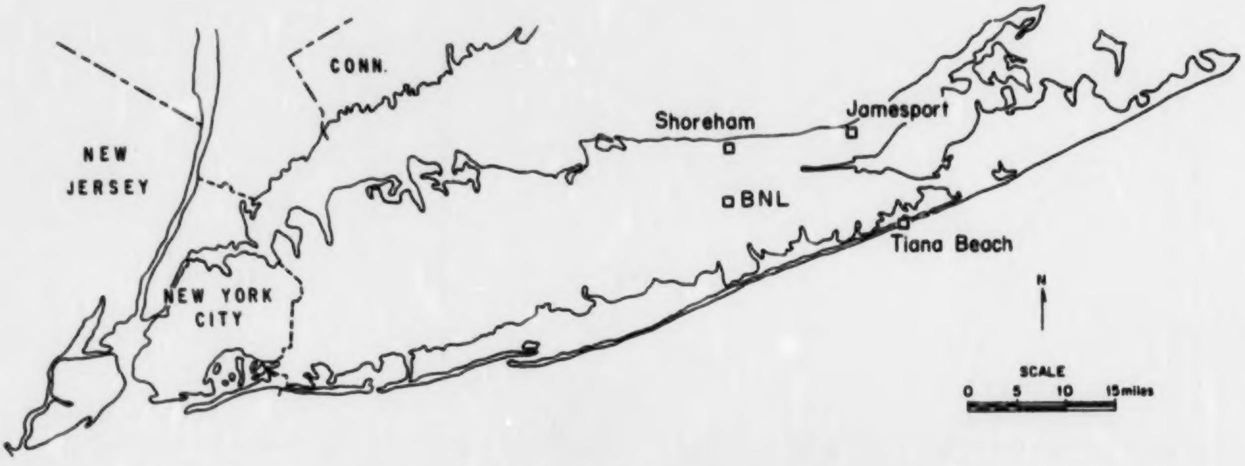
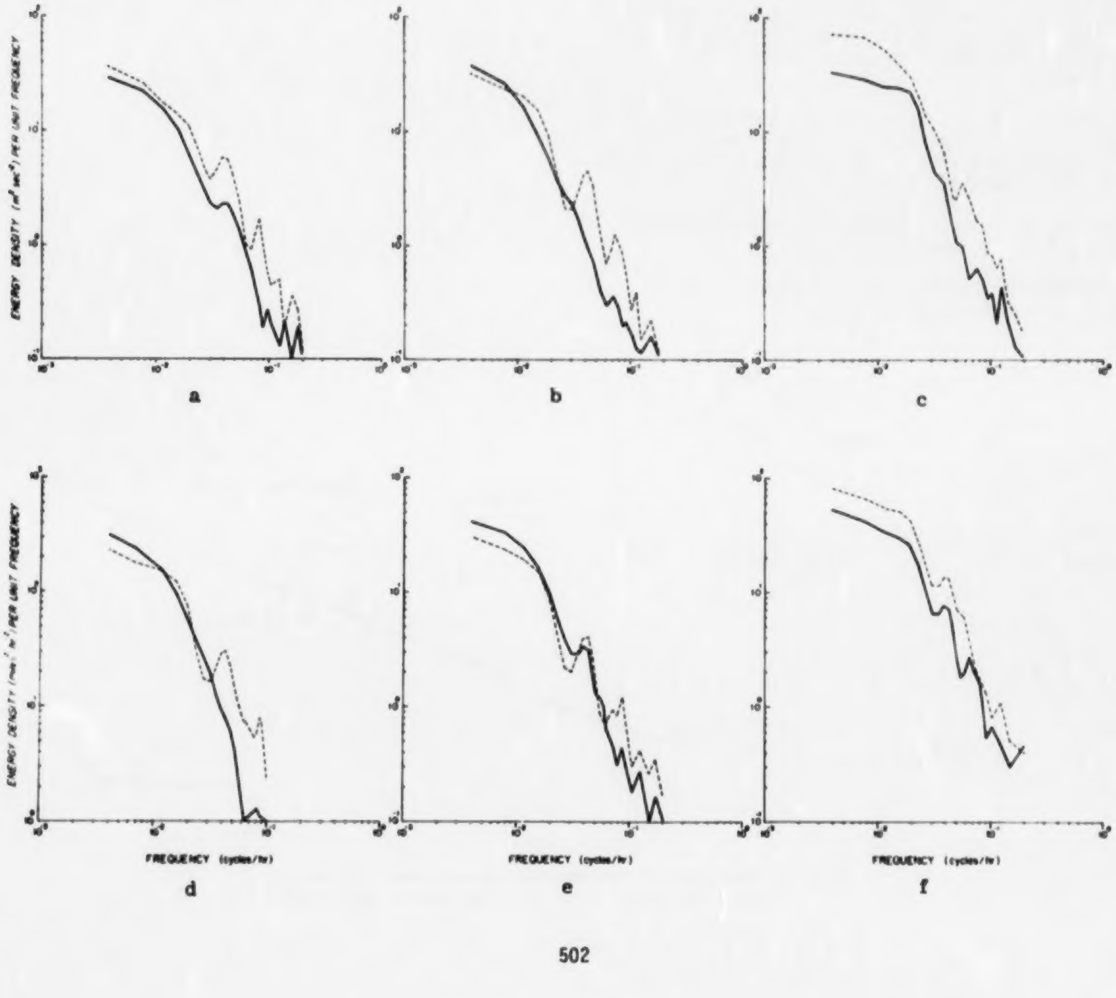


Fig. 1 Location of the specific measurement sites used for this study on Long Island, New York.

Fig. 2 Rotary Spectral Density Estimates:
- a) Spectrum of the horizontal wind during summer at Tiana Beach at the 75 ft. level.
- b) Spectrum of the horizontal wind during summer at Brookhaven National Laboratory at the 355 ft. level.
- c) Spectrum of the horizontal wind during winter at Brookhaven National Laboratory at the 355 ft. level.
- d) Spectrum of the horizontal wind during summer at Jamesport at the 400 ft. level.
- e) Spectrum of the horizontal wind during summer at Shoreham at the 33 ft. level.
- f) Spectrum of the horizontal wind during summer at Shoreham at the 150 ft. level.

The solid lines represent the anticlockwise spectrum and the dashed lines the clockwise spectrum. If S(f) is the true spectral estimate and S_f is the estimated value, then there is a 90% confidence (for 10 degrees of freedom set by a chi-squared distribution) that $0.55\ S_f < S(f) < 2.5 S_f$ (Gossard and Noonkester[3]).



A NUMERICAL MODEL FOR STABLY STRATIFIED FLOW AROUND COMPLEX TERRAIN*

James J. Riley
Hsien-Ta Liu
Edward W. Geller
Flow Research, Inc.
Kent, Washington

Summary

A computer program has been developed, based on an expansion suggested by Drazin (1961)[1] and Lilly (1973)[2] to compute three-dimensional stratified flow around complex terrain for the case of very strong stratification (small internal Froude number). Also, laboratory experiments were performed for strongly stratified flow past three different terrain models. Preliminary comparisons of the results of the computer program and the laboratory modeling indicate that the computed results are in fair agreement with the experiments. Discrepancies are probably attributable mainly to the separated wake in the lee of the models. Other possible sources of error are discussed in some detail.

1. Introduction

Assessment of the environmental impact of the release of pollutants into the atmosphere involves the estimation of diffusion patterns under atmospheric conditions ranging from average to extreme. A detailed knowledge of the wind field is important in the estimation of diffusion patterns, especially if the region of release is characterized by complex terrain. Thus, in the assessment of pollution effects, the understanding and prediction of local wind fields is often very important.

One approach to understanding and predicting local wind fields is numerical simulation. However, the numerical simulation of three-dimensional stratified flow over complex terrain is a very difficult task. This difficulty is a result of numerical complications associated with stratification effects and complex boundaries, and also of the limitations imposed by the core size and cycle time of present day computers. Thus, exploration of certain limiting conditions under which the physical, mathematical and numerical problems can be simplified is useful. One such limit is that of very large internal Froude number, i.e., weak stratification, where the tools of three-dimensional potential-flow theory are often available. Another limit is very small internal Froude number, or strong stratification.

When fluid is strongly stably stratified, vertical motions are heavily constrained and fluid elements tend to remain in their horizontal planes. The degree to which they do remain is measured by the ratio of their initial kinematic energy, $\frac{1}{2}\rho_o U^2$, to the potential energy required to lift the fluid element over or around the obstacle,

$$-\frac{1}{2}\, g \,\frac{d\bar{\rho}_c}{dx_3}\, h^2 .$$

Here, h is the characteristic vertical scale of the obstacle, g is the acceleration due to gravity, and $\frac{d\bar{\rho}_c}{dx_3}$ is a characteristic ambient stratification. The ratio is

$$-\frac{\rho_o U^2}{g\,\frac{d\bar{\rho}_c}{dx_3}\,h^2} = \left(\frac{U}{Nh}\right)^2 = F^2 ,$$

the square of the internal Froude number, where

$$N = \sqrt{-\frac{g}{\rho_o}\frac{d\bar{\rho}_c}{dx_3}}$$

is a characteristic Brunt-Vaisala frequency of the ambient fluid. For strongly stratified flows ($F \to 0$), Drazin (1961)[1] and, later, Lilly (1973)[2] have proposed a formal expansion in F^2, which predicts that to the lowest order, the flow resembles two-dimensional (horizontal) flow around contours of terrain at a given level. The deviations from this two-dimensional flow can be determined from the higher order terms in a power series.

In the work discussed in this presentation, we have developed computer programs to solve the equations resulting from the expansion suggested by Drazin and Lilly. We have also performed laboratory studies of stratified flows past simple terrain configurations to validate the numerical programs. Finally, we have made preliminary comparisons of theory and experiment.

2. Brief Description of the Theory

Consider the steady-state flow past a three-dimensional terrain feature with a typical vertical scale, h, and horizontal scale, L. We assume the oncoming (free-stream) flow has characteristic velocity, U, and characteristic stratification, $d\bar{\rho}_c/dx_3$, which is a constant. (The coordinate system is oriented with positive x_3 vertically upwards). We will also make the Boussinesq approximation and will neglect viscous (turbulent) effects. The equations of motion are (see Phillips, 1966)[3]:

$$\underset{\sim}{\hat{u}} \cdot \hat{\nabla}\underset{\sim}{\hat{u}} = -\frac{1}{\rho_o}\,\hat{\nabla}\hat{p} + \frac{\hat{\rho}}{\rho_o}\,\underset{\sim}{g} \qquad \underset{\sim}{g} = (0,0,-g) \qquad (2.1)$$

$$\hat{\nabla} \cdot \underset{\sim}{\hat{u}} = 0 \qquad (2.2)$$

and

$$\underset{\sim}{\hat{u}} \cdot \hat{\nabla}\rho + \hat{u}_3\,\frac{d\hat{\bar{\rho}}}{d\hat{x}_3} = 0. \qquad (2.3)$$

Here, $\hat{\underset{\sim}{u}}$ is the velocity vector, $\hat{\rho}$ is the density fluctuation about the ambient $\bar{\rho}$, and $\hat{p}$ is the pressure perturbation about the ambient. The vertical displacement of a fluid element, $\hat{\psi}$, is given by

$$\underset{\sim}{\hat{u}} \cdot \hat{\nabla}\hat{\psi} = \hat{u}_3 . \qquad (2.4)$$

Following Lilly (1973)[2], we scale the variables as follows:

$$\underset{\sim}{u}_H = \frac{\hat{\underset{\sim}{u}}_H}{U}\,,\quad \underset{\sim}{x}_H = \frac{\hat{\underset{\sim}{x}}_H}{L}\,,\quad x_3 = \frac{\hat{x}_3}{h}\,,\quad p = \frac{\hat{p}}{\rho_o U^2}\,, \qquad (2.5a,b,c,d)$$

where the subscript, H, denotes the horizontal component of a vector. To scale $\hat{\rho}$, we assume that

$\frac{1}{\rho_o}\frac{\partial\hat{p}}{\partial\hat{x}_3}$ and $\frac{\hat{\rho}}{\rho_o}\,g$ are in approximate (hydrostatic) balance in the vertical momentum equation. Then,

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$$\rho = \frac{\hat{\rho}}{\left(\rho_o U^2\right)/\left(gh\right)} \qquad (2.5e)$$

To scale $\hat{u}_3$, we assume that $\hat{u}_3 \frac{d\hat{\bar{\rho}}}{dx_3}$ and either $\hat{u}_1 \frac{\partial\hat{\rho}}{\partial\hat{x}_1}$ or $\hat{u}_2 \frac{\partial\hat{\rho}}{\partial\hat{x}_2}$ (or both) are in approximate balance in equation (2.3), which results in

$$u_3 = \frac{\hat{u}_3}{U \frac{h}{L} F^2} , \qquad (2.5f)$$

where

$$F = \frac{U}{Nh} \qquad (2.6a)$$

is the Froude number,

$$N = \sqrt{- \frac{g}{\rho_o} \frac{d\bar{\rho}_c}{dx_3}} \qquad (2.6b)$$

is the characteristic Brunt-Vaisala frequency, and where we scale the ambient stratification (assumed) horizontally uniform as

$$\frac{d\bar{\rho}}{dx_3} = \frac{d\hat{\bar{\rho}}}{dx_3} \bigg/ \frac{d\bar{\rho}_c}{dx_3} . \qquad (2.6c)$$

From (2.4), the scaling for $\hat{\psi}$ is

$$\psi = \frac{\hat{\psi}}{hF^2} . \qquad (2.6d)$$

Substituting (2.5) into the horizontal component of (2.1), we find

$$\underline{u}_H \cdot \nabla\underline{u}_H + F^2 u_3 \frac{\partial}{\partial x_3} \underline{u}_H = - \nabla_H p . \qquad (2.7)$$

The vertical component of (2.1) becomes

$$\left(\frac{h}{L}\right)^2 F^2 \underline{u}_H \cdot \nabla u_3 + \left(\frac{h}{L}\right) F^4 u_3 \frac{\partial}{\partial x_3} u_3 = - \frac{\partial p}{\partial x_3} - \rho \qquad (2.8)$$

Continuity is now expressed as

$$\nabla \cdot \underline{u}_H + F^2 \frac{\partial u_3}{\partial x_3} = 0 , \qquad (2.9)$$

and the incompressibility condition is

$$\underline{u}_H \cdot \nabla\rho + F^2 u_3 \frac{\partial\rho}{\partial x_3} - u_3 \frac{d\bar{\rho}}{dx_3} = 0. \qquad (2.10)$$

Finally, the equation for ψ, the displacement, becomes

$$\underline{u}_H \cdot \nabla\psi + F^2 u_3 \frac{\partial\psi}{\partial x_3} = u_3 . \qquad (2.11)$$

Next, we expand the independent variables in the powers of the small parameter, $\varepsilon = F^2$, i.e.,

$$(\underline{u}_H, u_3, p, \rho, \psi) = \sum_{n=0}^{\infty} \varepsilon^n \left(\underline{u}_H^{(n)}, u_3^{(n)}, p^{(n)}, \rho^{(n)}, \psi^{(n)}\right). \qquad (2.12)$$

The resulting equations to the lowest order are

$$\underline{u}_H^{(o)} \cdot \nabla\underline{u}_H^{(o)} = - \nabla_H p^{(o)} , \qquad (2.13)$$

$$\nabla \cdot \underline{u}_H^{(o)} = 0, \qquad (2.14)$$

$$\frac{\partial p^{(o)}}{\partial x_3} = - \rho^{(o)} , \qquad (2.15)$$

$$\underline{u}_H^{(o)} \cdot \nabla\rho^{(o)} - u_3^{(o)} \frac{d\bar{\rho}}{dx_3} = 0, \qquad (2.16)$$

and

$$\underline{u}_H^{(o)} \cdot \nabla\psi^{(o)} = u_3^{(o)} . \qquad (2.17)$$

Combining (2.16) and (2.17) gives

$$\underline{u}_H^{(o)} \cdot \nabla\left[\rho^{(o)} - \psi^{(o)} \frac{d\bar{\rho}}{dx_3}\right] = 0.$$

Assuming $\rho^{(o)}$ and $\psi^{(o)}$ are zero in the free stream, then, since $\frac{d\bar{\rho}}{dx_3}$ is independent of $\underline{x}_H$, one obtains

$$\rho^{(o)} = \psi^{(o)} \frac{d\bar{\rho}}{dx_3} ,$$

or with (2.15)

$$\psi^{(o)} = - \frac{\partial p^{(o)}}{\partial x_3} \bigg/ \frac{d\bar{\rho}}{dx_3} . \qquad (2.18)$$

Note that, from equations (2.13) and (2.14), the equations for $\underline{u}_H^{(o)}$ and $p^{(o)}$ are those for an inviscid, two-dimensional flow in a horizontal plane. In particular, if the incoming (horizontal) flow is irrotational, then the entire horizontal flow field is irrotational. Thus, in this case the tools of the potential-flow theory can be employed to compute the flow. In a given horizontal plane, the resulting solution would be that of a two-dimensional flow about an obstacle defined by the contour of the terrain at the vertical level of that terrain. The vertical displacement can be computed from (2.18), where it is a result of the pressure difference in the flow between two adjacent horizontal layers. A calculation of the vertical displacement can also be used to estimate the region of validity of the results.

Equations (2.13), (2.14) and (2.18) were programmed on the computer for flow past somewhat arbitrarily shaped terrain features. The free-stream flow was assumed irrotational, and standard numerical procedures for computing the two-dimensional potential flow past arbitrarily shaped bodies were used.

3. Description of the Experiment

The experimental setup was basically the same as that discussed in Flow Research Report No. 57 (Liu and Lin, 1975)[4]. In addition to the idealized terrain model, which has been used for detailed studies in the past (see Flow Research Report No. 29)[5] and is defined by

$$h_I(\hat{x}_1,\hat{x}_2) = 17.8 \Big\{ \exp\Big[-.0008513(\hat{x}_1 - 61)^2 - .01197 (\hat{x}_2 - 18.82)^2\Big] + \exp\Big[-.0008513(\hat{x}_1 - 61)^2 - .01197(\hat{x}_2 + 18.82)^2\Big]\Big\} + 16\Big\{\exp\Big[-.01171(\hat{x}_1 - 61)^2 - .002314 \hat{x}_2^2\Big]\Big\} , \qquad (3.1)$$

we used a conically shaped model

$$h_C(\hat{x}_1,\hat{x}_2) = \begin{cases} 30 \left(1 - \frac{r}{15}\right) & r \le 15 \\ 0 & r > 15, \end{cases} \qquad (3.2)$$

and a Gaussian shaped model,

$$h_G(\hat{x}_1,\hat{x}_2) = 30 \exp\left[-\left(\frac{r}{20}\right)^2\right]. \qquad (3.3)$$

Here, $r = \left(x_1^2 + x_2^2\right)^{1/2}$ and all distances are measured in centimeters.

The two latter (new) models were designed to be interchangeable with the idealized model. Neutrally buoyant dyes, each of a different color, were released through small stainless-steel tubes (.3 mm I.D.) at three levels upstream of the model. Three plumes spaced in the horizontal were released in each level. The plume trajectories were photographed, and then analyzed for later comparisons with analytical results. Figure 1 shows a typical side view of the streak-line patterns for flow past the Gaussian peak.

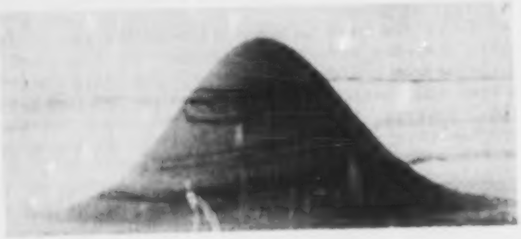

Figure 1. The Flow Patterns Traced by Neutrally Buoyant Dye in the Vicinity of a Three-Dimensional Gaussian-Shaped Model. N = .135 Hz, U = 4 cm/s, F_h = .97.

Note that in each horizontal plane, three streak lines were released. However, in the side view, the three are difficult to distinguish, especially in the lowest Froude number cases. This difficulty is somewhat compounded by the slight vertical spread of each streak line. However, in a given horizontal plane, the innermost streak line is displaced more than the others, so that its displacement is easily detectable in the photographs. Thus, when comparisons were made, we used the innermost streak line.

The choice of the model conditions was based on the following criterion. The expansion can only remain valid as long as streamlines do not cross in the vertical. This crossing would occur, for example, if $\hat{\psi}(\hat{x}_3) > \hat{\psi}(\hat{x}_3+\Delta\hat{x}_3)+\Delta x_3$. Thus, $-\Delta\hat{x}_3 > \hat{\psi}(\hat{x}_3+\Delta\hat{x}_3)-\psi(\hat{x}_3)$, or in the limit, as $\Delta\hat{x}_3 \to 0$,

$$-\frac{\partial\bar{\psi}}{\partial x_3} \geq 1.$$

When one considers both upward and downward displacements, this condition generalizes to

$$\left|\frac{\partial\bar{\psi}}{\partial x_3}\right| \geq 1.$$

Thus, in nondimensional terms, a necessary condition for the validity of the expansion is

$$F^2\left|\frac{\partial\psi}{\partial x_3}\right| \leq 1. \qquad (3.4)$$

We selected the various parameters in the experiments so that (3.4) was satisfied over a large portion of the vertical region of interest. The Froude number range of the experiments was roughly from .05 to .5.

4. Comparisons of Experimental and Numerical Results

The general behavior of the streak lines can be seen by examination of figure 1 . In the middle horizontal plane, consider the inner streak line, which exhibits the largest vertical displacement. As a fluid element approaches the model, it slows down in a manner similar to an element in a two-dimensional flow about a cylinder. Simultaneously, the element experiences an upward pressure force, causing it to rise upward (see equation 2.18). As the element starts around the mountain, it accelerates, the vertical pressure force changes direction, and the element is displaced downward. The flow separates near the point of maximum lateral extension of the model. Past the midpoint of the mountain, the elements return to their equilibrium levels, and are entrained into the wake of the model. For the Froude number range in the experiments, the wake flow in the lee of the model appeared to consist of turbulent, quasi-horizontal eddies, whose vertical velocity fluctuations were rapidly decaying with downstream distance.

The incoming flow was slightly unsteady. We observed that the inner streak lines slowly oscillated from one side of the mountain to the other. This oscillation often produced an inner streak-line pattern as sketched in figure 2.

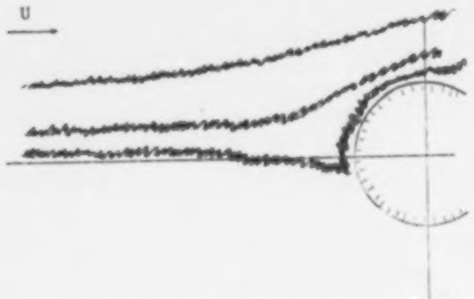

Figure 2. Sketch of the Instantaneous Streak-Line Pattern

One possible explanation of this phenomenon is the following. For two-dimensional flow past a cylinder, turbulent vortex streets are observed in the Reynolds number range of about $60 \leq R \leq 5000$, where the Reynolds number R is UD/ν, D is the diameter of the cylinder, and ν is the kinematic viscosity. For our case, R is typically

$$R \approx \frac{4\text{ cm/sec} \times 10\text{ cm}}{.01\text{ cm}^2/\text{sec}} \approx 4000\ ,$$

which is in this range. The vortex motion is accompanied by movement of the stagnation points, which in turn causes the incoming flow to oscillate slightly. For R in this range, the Strouhal number, defined by S = nD/U, where n is the vortex shedding frequency in radians/sec, is approximately .21. Thus,

$$\frac{n}{2\pi} \approx \frac{.21 \times 4\text{ cm/sec}}{2\pi \times 10\text{ cm}} \approx .014\text{ cycles/sec.}$$

This value corresponds roughly to the frequency of the oscillations noted in the experiments.

Figure 3 shows streak lines in the horizontal plane, x_3 = 13.2 cm (the middle plane) for the Gaussian model with F = .152. Also shown are the numerical predictions. In addition, the contour of the model at the free-stream level of the plumes is displayed. Note that the numerical calculation tends to underpredict streakline displacement. This discrepancy is probably the result of mainly two effects. The first is the displacement effect of the boundary layer, which is not taken into account in the inviscid numerical model. The second and more important effect is the displacement effect of the separated wake. These two effects together produce an "apparent" body, as sketched in figure 4a.

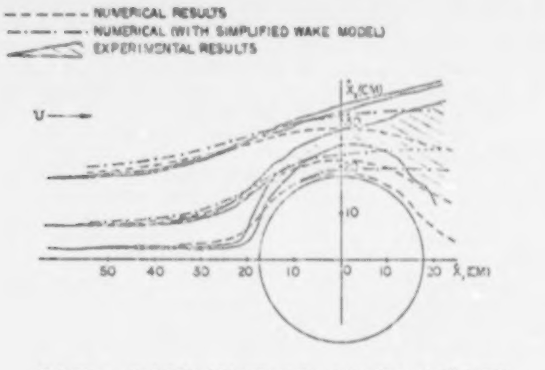

FIGURE 3. COMPARISON OF EXPERIMENTAL & NUMERICALLY COMPUTED STREAK LINES IN THE HORIZONTAL PLANE DEFINED BY $\hat{x}_3$=14 CM FOR CASE V C (GAUSSIAN MODEL F_R =.90)

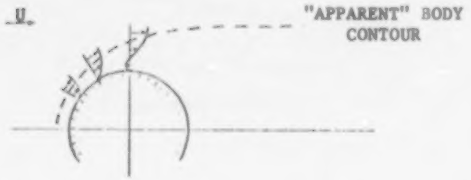

Figure 4a. Apparent Body Shape

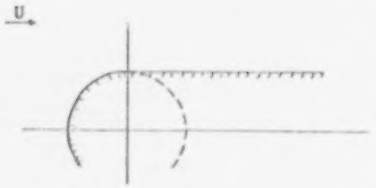

Figure 4b. Model for the Separated Wake

Note that for a two-dimensional flow past a circular cylinder, if the Reynolds number is subcritical (i.e., below approximately 3×10^5), the boundary layer is laminar, and it separates at about 80° from the front stagnation point (Schlichting, 1960)[6]. Since the Reynolds numbers for the experiments were an order of magnitude less than the critical value, it is reasonable to assume that the boundary layer was laminar and separated before the point of maximum lateral extension of the body. For two-dimensional flow past a circular cylinder, if the Reynolds number is supercritical, the boundary layer is turbulent, and separation probably occurs just past the point where the cross section starts to converge. Thus, in the full-scale case, where Reynolds numbers will usually be several orders of magnitude larger than the critical value, separation is likely to occur just past the point of maximum lateral extent.

When viscous terms are added to the scaling arguments presented in section 2, one finds that the lowest order solution is no longer two-dimensional. Thus, the conclusions drawn above could be modified somewhat because of the three-dimensional nature of the boundary layer.

The displacement effect of the separated wake was crudely modeled by extending the body, as shown in figure 4b. Figure 3 also shows the results of a calculation using this body shape instead of the circular shape. The modification of the streak lines, especially the outermost ones, is noticeable. However, from the discussion above, the model suggested in figure 4b is probably more adequate for the full-scale case than the laboratory case. Also, the effect of the boundary layer may have to be taken into account to obtain close agreement between the numerical and experimental results.

The width of the tank is approximately 120 cm, so it is possible that the sidewalls influence the flow field near the models. Sidewalls were not included in the numerical calculations for the Gaussian and conical models. However, the horizontal displacement of the streamline whose free-stream position is at the sidewalls was computed. For the Gaussian and conical models, the displacement of this streamline was negligible for the cases computed. Thus, for these cases, we can assume that the effect of sidewalls is unimportant.

Figure 5 shows the experimentally determined vertical displacement for the conical model with F = .109. Also shown in this plot is the numerical prediction for the innermost plume in the middle level. The numerical calculation predicts a very slight rise in the plume as it approaches the mountain, which is also discernible in the experiments. The distance that the plume drops is also predicted fairly well. However, the asymmetry of the experimental results is missed entirely. This discrepancy is again probably attributable to the neglect of the boundary layer and wake effects.

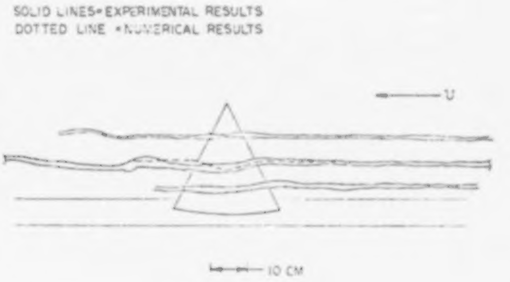

FIGURE 5 COMPARISON OF EXPERIMENTAL & NUMERICALLY COMPUTED RESULTS FOR VERTICAL DISPLACEMENT FOR CASE IX b (CONICAL MODEL F_R =.74)

Figure 6 shows similar experimental plots for the Gaussian model at F = .152. Also shown are the numerical predictions for the innermost plume for each of the three levels. The agreement and explanation of the results are very similar to the previous case.

Finally, figure 7 shows comparisons of experimentally observed and numerically computed streak lines for the idealized terrain case, with F = .218. The dye was released at approximately $\hat{x}_3$ = 11.5 cm. Note that the

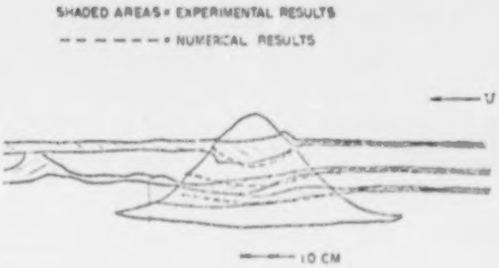
SHADED AREAS = EXPERIMENTAL RESULTS
- - - - - - - = NUMERICAL RESULTS
U
10 CM

FIGURE 6. COMPARISON OF EXPERIMENTAL & NUMERICALLY COMPUTED RESULTS FOR VERTICAL DISPLACEMENT FOR CASE IV C (GAUSSION MODEL, Fr = .97)

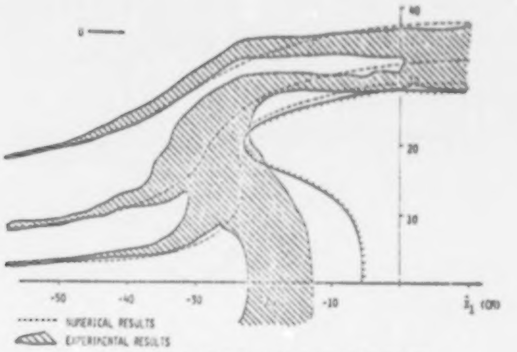

FIGURE 7. COMPARISON OF EXPERIMENTAL & NUMERICALLY COMPUTED STREAK LINES IN THE HORIZONTAL PLANE DEFINED BY $\hat{x}_3$ = 11.5 CM (IDEALIZED TERRAIN MODEL. F_o = 1.37)

calculation included separation in the wake, as discussed above. Comparisons for this case are much better than for the previous cases because the crude wake modeling for the potential flow calculation closely matched the real flow. In the calculations for the previous cases, the assumption that the separation stream line is straight and parallel to the upstream flow direction was not supported by the experimental results which indicate a diverging wake region.

An examination of the side view shows sizeable vertical displacement as the stream lines traverse the ridge. This is accompanied by some motion towards the ridge, resulting in the inner plume appearing to cut through the terrain in the top view. As the fluid comes over the ridge, it tends to fall below its ambient level, thus forcing the fluid laterally away from the ridge, and producing the slight bulge seen in the figure above the ridge. This bulge may also be attributable to a boundary layer separation bubble. According to the potential flow calculation, the boundary layer is subjected to an adverse pressure gradient near the most upstream point on the model. Therefore, separation of the laminar boundary layer is likely.

Finally, calculations of the streamline at the location of the tank sidewall show that its lateral displacement is significant. Thus sidewall effects, which were neglected in the calculation, could be of some importance in this case.

5. Conclusions and Suggestions for Future Studies

This study was intended to be a very preliminary examination of the use of the scaling suggested by Drazin (1961)[1] and Lilly (1973)[6] for the case of very low Froude-number, three-dimensional flow over complex terrain. Preliminary results indicate the following:

(i) For the Froude number regime studied, the basic scaling suggested was appropriate, and the flow did resemble two-dimensional flow around contours of the terrain model at the appropriate level.

(ii) To improve the numerical model, the inclusion of at least two effects is of primary importance. They are: (a) the displacement effect of the boundary layer, and, more importantly, (b) the displacement effect of the separated wake.

(iii) The prediction of vertical displacement was roughly valid for the case computed, considering that the effects discussed in (ii) were not modeled.

(iv) The accuracy of the lowest order solution depends strongly on the type of terrain feature considered, as well as the vertical level, the lateral distance from the terrain feature, and, of course, the Froude number. For a given Froude number, the agreement between the numerical model and experiment was much better for the idealized complex peak than for the Gaussian and conical models.

(v) The computed vertical displacement can be used to estimate regions of applicability of the lowest order solution.

(vi) Slight unsteadiness in the oncoming flow may be a result of turbulent vortex shedding in the lee of the models.

One obvious improvement can be made in the numerical model. The separated wake can be crudely modeled by standard techniques used in aerodynamics to compute flow past two-dimensional bodies. (Note, however, that one may have to take into account the three-dimensional nature of the boundary layer).

Several other improvements are also possible. First, one could include the vertical and horizontal shearing of the free-stream flow. Second, the atmospheric boundary layer could be modeled. This modeling can be accomplished most simply by using the computed inviscid flow to derive a turbulent boundary layer model. A more sophisticated approach would allow the computed boundary layer to react back on the inviscid flow. Third, the scaling analysis could include the effect of atmospheric compressibility, although this effect shouldn't be too important because the vertical motions are weak. Fourth, Coriolis forces could be included. Fifth, as discussed by Drazin and Lilly, the scaling breaks down near the model peaks (because the local scale height is very small, and, therefore, the local Froude number is very large). An investigation of the coupling of the present numerical model with some other model near the mountain peaks could be performed. Sixth, turbulent diffusion could be modeled in the plume dispersion process with the turbulent diffusivity related to the local Richardson number. Finally, it is implicit in the scaling analysis that $d\bar{\rho}_c/dx_3$ characterize the complete density profile. For example, in regions where $d\tilde{\rho}/d\tilde{x}_3$ is very small compared to $d\bar{\rho}_c/dx_3$, the expansion will probably break down. So the case of a two-layer fluid (each layer having a different constant density) cannot be treated with the present scaling. Thus, rescaling the equations to include these more general cases would be useful.

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HYDRODYNAMIC AND WATER QUALITY MODELING IN THE OPEN OCEAN USING MULTIPLE GRID SIZES

Priya J. Wickramaratne, James W. Demenkow,
Stanley G. Chamberlain and Janice D. Callahan
Environmental, Systems Analysis
Oceanographic & Environmental Services
Raytheon Company
Portsmouth, Rhode Island

ABSTRACT

This paper discusses the problems and limitations of the application of hydrodynamic and water quality models to open ocean areas in which varying degrees of resolution are required. In applications involving power plant or wastewater treatment discharge into large bodies of water, a higher degree of spatial resolution is often required near the discharge location. The models have been executed using two different grids sizes in order to obtain the desired resolution while reducing overall computer costs. The grids were intermeshed using a technique in which the length scale of the larger grid was an even multiple of the smaller grid. The results obtained using the larger grid were used to generate boundary conditions for the smaller grid. This was easily accomplished since the length scale of the larger grid was taken to be an even multiple of the smaller grid.

INTRODUCTION

The modeling of environmental problems pertaining to water pollution frequently requires a greater level of detail in certain geographical regions, while not requiring as much in the rest of the study area. For example, a model of a discharge plume would require considerably more detail in the vicinity of the outfall, where the concentration gradients are the steepest, and less detail as one moves away from the outfall, where the gradients are considerably less steep.

Many of these water quality models use a finite difference technique, where the study area is overlaid by a grid of constant cell size. Computer costs and core storage size often make the modeling of the entire area with a grid fine enough to obtain the desired details both costly, and impractical. Hence, the need exists to mesh together a fine and coarse grid structure which will provide both the desired detail of the fine grid and the economic advantages of the coarse grid.

This paper describes a technique to accomplish the intermeshing of coarse and fine grid structures in far-field models for any well-mixed waterway. An application of the technique is given to illustrate how it can be performed for an open ocean situation.

TECHNIQUES

Circulation Model

A circulation model used extensively by Raytheon is a two-dimensional long wave propagation model based on Leendertse[1].

The model consists of a digital computer algorithm which yields a numerical solution to the vertically - averaged hydrodynamic equations of motion. The equations of motion describe water currents which are driven by horizontal pressure gradients produced by tidally induced changes in surface elevation.

They include a "continuity equation"

$$\frac{\partial \eta}{\partial t} + \frac{\partial (h+\eta)}{\partial x} + \frac{\partial (h+\eta)}{\partial y} = 0$$

and the momentum equations

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial \eta}{\partial x} + g\frac{u(u^2+v^2)^{1/2}}{C^2(h+\eta)} = 0$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial \eta}{\partial y} + g\frac{v(u^2+v^2)^{1/2}}{C^2(h+\eta)} = 0$$

where:

u = vertically-averaged velocity in x direction.
v = vertically-averaged velocity in y direction.
η = incremental tide height about mean value.
h = water depth to reference plane (mlw).
C = Chezy coefficient.
g = acceleration of gravity.
t = time.

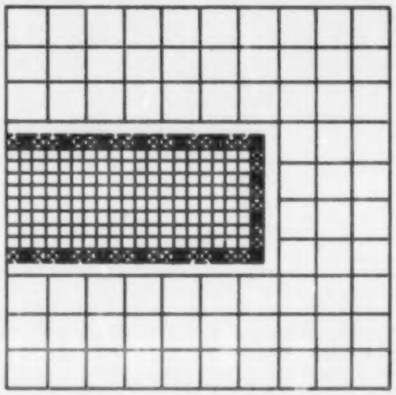
These equations are solved numerically by the multi-operation method[1] which possesses the good stability attributes of a pure implicit scheme and the computational efficiency of an explicit scheme.

Boundary Conditions. A key to running the circulation model is the generation of the appropriate driving forces on the boundaries. This paper will concentrate on the generation of boundary conditions at the boundaries between the coarse and fine grid regions. (The outer boundary conditions for the coarse grid region are specified in the usual way).

If the fine grid region is entirely within the coarse grid region, as in Figure 1, then the fine grid boundary conditions can be found from the coarse grid simulation. Boundary condition data for the fine grid is obtained by first executing the coarse grid model and saving the computed water levels in the cells which form the boundaries of the fine grid, at every time step over the desired simulation time period. The values thus obtained, are linearly interpolated between spatial points (at every time step), as shown in Figure 1, to give the desired boundary conditions. The time step is determined from the grid size and water depth, with computer costs being used as constraints, to satisfy the accuracy criterion,

$$\Delta t \leq 2\Delta L\ (gh)^{-1/2}$$

where Δt is the time step, and ΔL is the length of a grid square.



---- Interfacial boundary - Coarse Grid Outside, Fine Grid Inside

• Boundary Values from Coarse Grid

x Interpolated Fine Grid Boundary Values.

Figure 1. Interfacial Boundary Within Fine and Coarse Grid Regions for Circulation Model.

Let ΔL_c be the length of the coarse grid, and ΔL_f be the length of the fine grid. In order to satisfy the accuracy criterion, a decrease in grid size from ΔL_c to ΔL_f would normally necessitate a decrease in time step Δt.

Let Δt_c be the time step used in the coarse grid and Δt_f be the time step used in the fine grid, where $\Delta t_f \leq \Delta t_c$. The boundary values obtained for the fine grid at time intervals of Δt_c, are linearly interpolated in time, to give values at time intervals of Δt_f.

Initial Conditions. Initial conditions for the fine grid area are obtained by saving the initial coarse grid values of water levels, and U and V velocities corresponding to the fine grid area, and performing a linear interpolation of the coarse grid values in the longitudinal and transverse directions and averaging these values.

Water Quality Model

A Raytheon water quality model used in conjunction with the above circulation model, is a digital computer model of the two-dimensional, time-varying advection and diffusion characteristics of a vertically well-mixed water body[2-6]

The basic equation which describes the dependence of the concentration (C) on the distance variables (x,y), time (t), depth (h), currents (U,V), constituent decay coefficient (k), diffusion coefficient (E_x, E_y) and discharge rate (S) is:

$$\frac{\partial (hc)}{\partial t} = \frac{\partial (hUC)}{\partial x} - \frac{\partial (hVC)}{\partial y} + \frac{\partial}{\partial x}\left[hE_x \frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial y}\left[hE_y \frac{\partial c}{\partial x}\right] - kC + S$$

The first five terms on the right-hand side of this equation represent, respectively, the x- and y-advection, x- and y-turbulent diffusion, and decay processes. The sixth term represents the effluent discharge rate. This is the basic conservation equation for a single constituent with each term representing the rate change of constituent concentration due to the particular processes. Additional terms can be added to the equation if the water quality constituent being modeled is linked to other constituents.

The numerical methods for solving the equation above are developed by discretizing the time and space variables to form a finite difference equation. A "forward difference" is used for rate of change of concentration with time and "central differences" are used for the diffusion terms. The finite differences for the advective terms are forward differences with respect to the direction of the currents, U and V, and are chosen to satisfy conservation of concentration in the discrete spatial volumes.

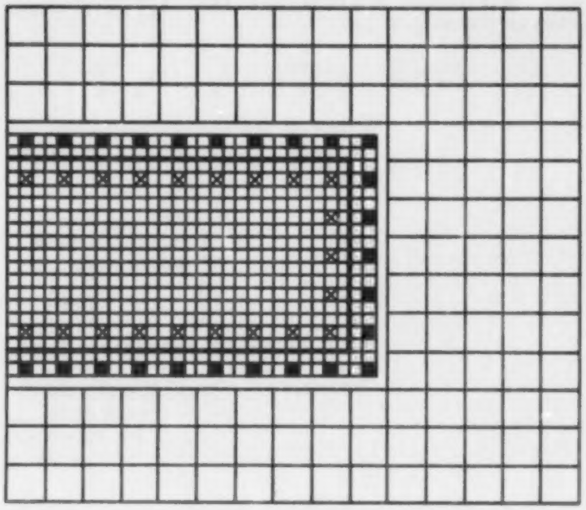
If the velocities generated by the circulation model are to be used as inputs to the water quality model, the grid layout for the water quality model must be the same as that for the circulation model.

Let ΔT_f be the time step used in the fine grid and let ΔT_c be the time step used in the coarse grid of the water quality model. (ΔT_c should be an exact multiple of ΔT_f, ΔT_c and ΔT_f (for water quality model) are not necessarily equal to Δt_c and Δt_f (for circulation model) but should be a multiple of them).

Starting with known initial conditions at some time t, the fine grid concentration values are computed first (since the source "box" is usually contained within the fine grid) over a time period (t, $t+n\Delta T_f$). The coarse grid concentration values are next computed for the same time period (t, $t+\Delta T_c$), with initial time equal to $t(\ n\Delta T_f = \Delta T_c)$.

The boundary values of the coarse grid and fine grid are then interchanged in the manner indicated in Figure 2. Since values computed at the boundaries are not generally as accurate as the interior values, the substitution of fine grid interior values for coarse grid boundary values, and vice versa, should

increase the accuracy of the boundary values for both grids.



---- Fine Grid Outer Boundary

-•-•- Coarse Grid Inner Boundary

• Boundary Values of Fine Grid From Coarse Grid

X Boundary Values of Coarse Grid from Fine Grid

Figure 2. Interfacial Boundaries Within Fine and Coarse Grid Regions for Water Quality Models.

This procedure is repeated for the desired length of the simulated time, with the boundary values of the fine and coarse grid being interchanged at contiguous intervals of time of length ΔT_c.

Since mass transfer occurs at the boundaries between the coarse and fine grid regions, the values of the concentrations in the coarse grid must be allowed to affect the values of the concentration in the fine grid and vice versa. This is the primary motivation for intermeshing the coarse grid and fine grid in the manner described.

APPLICATION

The techniques described in the preceding section are now illustrated by the application to the dispersion of a water quality constituent discharged into a coastal region.

Circulation Model

Grid Size The grid size was selected to give the desired spatial resolution of currents and realistic representation of boundary contours commensurate with computer costs and capacity. A coarse grid with a length of 1/3 nautical mile (2025 feet) between points was used to model the entire **survey area. A fine grid with a length of 1/9 nautical mile (675 feet) was used to obtain the necessary detail in the immediate vicinity of the discharge point (see Figure 3).**

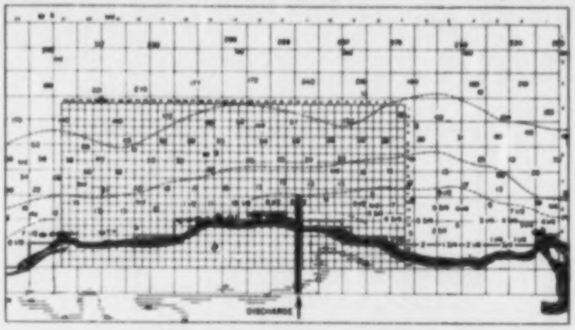


Figure 3. Fine and Coarse Grid Regions for Open Ocean Example

Time Step The time step for the coarse grid was chosen to be 60 seconds. Based on a sensitivity analysis (the fine grid was originally run with a time step of 20 seconds) the time step for the fine grid was also selected to be 60 seconds to minimize computer costs.

Boundary Conditions - Coarse Grid Tide heights were specified on all the open boundaries. The tide heights on the two boundaries perpendicular to the coast were determined from tidal measurements and tide heights from the nearest National Ocean Survey tide reference station. The tide heights along the boundary parallel to the coast were determined by linearly interpolating the values at the two end boundaries.

Boundary Conditions - Fine Grid The boundary conditions for the fine grid were computed by the coarse grid model. As shown in Figure 3, the outside boundary of the fine grid corresponds to a set of interior grid points in the coarse grid. The numbers computed along this interfacial boundary in the coarse grid were then used as input to the fine grid model.

Water Quality Model

The grid layout for the water quality model is the same as that for the circulation model (shown in Figure 3) for the coarse and fine grids. The ambient tidal currents (U,V) are obtained from the circulation model. The time step was selected as 15 minutes and 5 minutes for the coarse grid and fine grid, respectively.

These values were based on the stability criterion:

$$\max \left[|U| + |V| \right] \frac{\Delta t}{\Delta L} \leq 1$$

RESULTS

Circulation Model

The results of the application of the coarse grid/fine grid technqiues to the open ocean example are best exemplified in Figures 4 and 5. Instantaneous velocities for both grid sizes are displayed in Figure 4 for a time of left-flowing tidal currents. The use of the fine grid allows better delineation of the coastline with the resulting improvement of resolution near the shore where the currents are somewhat less (lead in phase) due to frictional effects. The fine grid displays the slower velocities quite nicely whereas the coarse grid does not.

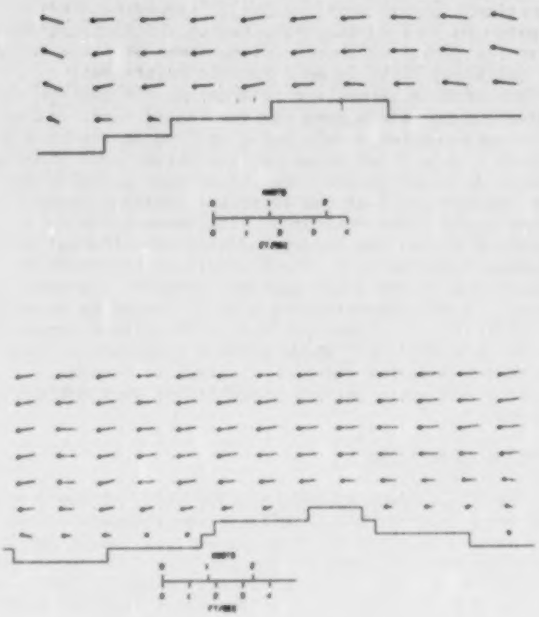
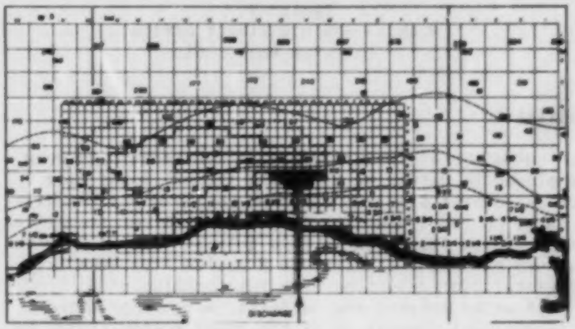


Figure 4. Instantaneous Coarse Grid (above) and Fine Grid (below) Currents for Time of Left Flowing Currents

Water Quality Model

Figure 5 displays the results of the water quality model. The need for improved resolution near the discharge can be seen by noting that the contour lines are less than three grid lines apart (the coarse grid resolution) over a large portion of the fine grid study area. Also, as noted from the left most portion of the 0.3 contour, the plume has sufficiently dispersed so that 1/9 mile resolution is no longer necessary beyond the fine grid region.



——1.0 Contour
----0.5 Contour
....0.3 Contour

Figure 5. Far Field Water Quality Distribution for Time of Maximum Leftward Plume

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BLACK RIVER THERMAL ANALYSIS

Donald R. Schregardus
U. S. Environmental Protection Agency
Region V
Michigan-Ohio District Office
Fairview Park, Ohio

Gary A. Amendola
U. S. Environmental Protection Agency
Region V
Michigan-Ohio District Office
Fairview Park, Ohio

ABSTRACT

One-dimensional temperature modeling techniques were employed to determine allowable thermal loads from United States Steel Corporation Lorain Works for discharge to the Black River. The Black River from river mile 5.0 to its mouth in Lake Erie at Lorain, Ohio is a complex system affected by dilution from Lake Erie, recirculation resulting from the location of U. S. Steel water intakes and outfalls, and abrupt changes in the physical dimensions of the river system caused by maintenance dredging by the U. S. Army Corps of Engineers. Based upon physical and hydrologic characteristics, the Black River below river mile 5.0 was divided into three segments. A one-dimensional thermal modeling technique was developed and applied to each segment taking into account river flow, lake dilution, meteorological data, and heat loadings from U. S. Steel. The equations were verified with measured data at critical stream flows and used to compute thermal loads which can be discharged by U. S. Steel and still meet applicable temperature standards. Practical considerations were employed in arriving at the final recommended effluent limitations.

BACKGROUND

The Black River is a system of natural drains flowing 23 miles in a generally northerly direction and emptying into Lake Erie at Lorain, Ohio. The State of Ohio has classified the river as a warm water fishery and correspondingly sets temperature standards to maintain this classification. The water quality standards for temperature applicable to the Black River limit the temperature increase of the river attributable to human activity to 5°F (2.8°C) and set maximum monthly water temperatures not to be exceeded. The above criteria are to be achieved at the water quality design flow of the stream which has been defined as the annual minimum seven-day consecutive flow with a recurrence interval of once in ten years. In the lower portion of the Black River the water quality design flow has been determined to be about 21 cfs.

The temperature regime in the lower portion of the river from mile 5.0 to its mouth at Lake Erie is affected by discharges from United States Steel Corporation's Lorain Works, a fully integrated steel plant. On July 23-26, 1974, Region V - Michigan-Ohio District Office conducted a comprehensive field survey on the Black River in an effort to determine the effect of U. S. Steel's discharges on the quality of water and to obtain data for verification of predictive mathematical models being applied to the river. Figure 1 is a location map of the survey area showing the U. S. Steel Lorain Works five river outfalls and two intakes and 8 of the 13 stream stations where water quality was monitored. The temperature data obtained during the survey indicate that thermal discharges from the U. S. Steel Lorain Works result in violations of the water quality standards presented above. Stream temperatures were increased by as much as 15°F by U. S. Steel outfalls with surface temperatures generally 12°F above ambient temperatures (temperatures measured above U. S. Steel). However, monthly allowable maximum temperatures were not exceeded.

GENERAL CONDITIONS

As the Black River approaches Lake Erie, stream level and water quality become affected by backwaters from the lake. Velocity profiles as well as sodium and chloride data obtained during the July 1974 survey and another U. S. EPA survey conducted on May 2, 1974, indicate that a wedge of cool lake water flows upstream along the bottom of the river beneath the warmer river and effluent water (See Figure 2). Further analysis of the data reveals that the intruding lake water causes dilution of river concentrations of sodium and chloride as far upstream as U. S. Steel intake WI-3 (RM 3.88). This lake water intrusion is a major component in the cooling of heated waters discharged to the lower portions of the stream.

Estimates of lake intrusion flow during the July survey were made using sodium and chloride data. Twenty-

FIGURE 1
BLACK RIVER LOCATION MAP

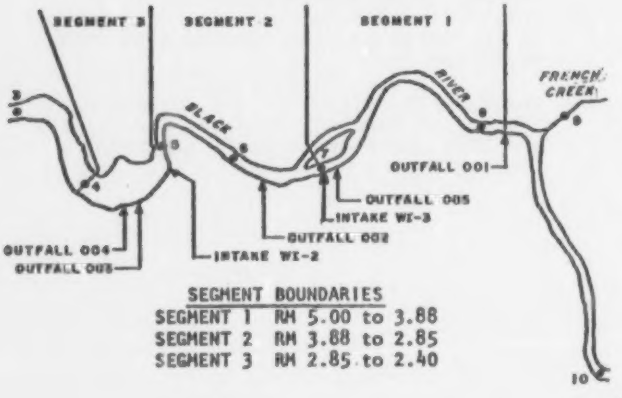
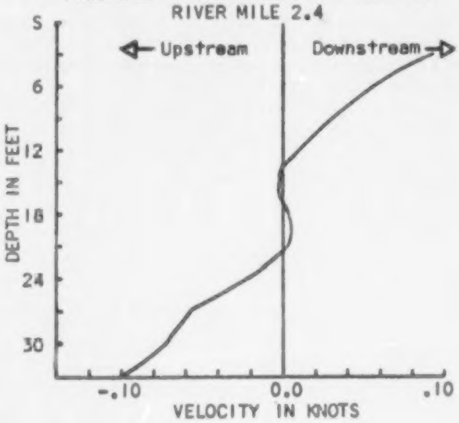


FIGURE 2 - STREAM VELOCITY PROFILE
RIVER MILE 2.4



four hour equal volume composite samples for sodium and chloride were obtained at top, middle, and bottom depths at five survey stations located between Outfall 001 and the downstream end of the turning basin (Figure 1). Because of the conservative nature of these elements and the large concentration differences between the river upstream of U. S. Steel and Lake Erie these data can be used in a mass equation to estimate the intrusion flow at each survey station. The computations are based upon the assumption that the instream quantities of both sodium and chloride are affected only by French Creek, discharges from U. S. Steel, and mixing with a known concentration of intrusion water. This assumption is reasonable in that the July survey was conducted during dry weather so that the runoff was negligible. In addition, stream and discharge flows and concentrations were relatively constant during the survey allowing the assumption of steady state conditions to be made. The resulting equation used to estimate the intrusion flow is:

$$Q_I = Q_R \frac{(C_R - C_m)}{(C_m - C_I)} \tag{1}$$

Where:

Q_R = river flow assuming no intrusion, cfs

C_R = expected river concentration assuming no intrusion flow, mg/l

C_m = measured concentration of the river, mg/l

C_I = concentration of the intruding water, mg/l

The daily intrusion flow at Stations 4, 5, 6, and 7 was determined by averaging the flow values computed using the sodium data and the chlorine data. This procedure was completed twice, once assuming the sodium and chloride concentration of the intruding water to be equal to the lake concentration and once assuming the concentration to be equal to the river concentration measured at the bottom of the next downstream survey station. The results of the computations are presented in Table 1. The computed intrusion flow at Station 4 using Station 3 bottom concentrations appears unreasonably high when compared with other data. Further review showed that Stations 3 and 4 have nearly the same concentrations causing the ratio of concentrations in Equation 1 to become very large. When concentrations are very close, small variations in the data can significantly alter the computed flow.

Based upon physical and hydrologic characteristics, the Black River below French Creek was divided into three segments, each with relatively uniform thermal properties (Figure 1). The upstream segment from Outfall 001 to Intake WI-3 (RM 5.0-3.88) was considered to be a one dimensional stream not yet affected by the intruding lake water. Segment 1 averages about 10 feet deep and 160 feet wide. Water withdrawn at Intake WI-3 is discharged at Outfalls 001 and 005. Heated water discharged at Outfall 001 cools as it flows downstream.

The second segment is located between the turning basin and Intake WI-3 (RM 3.88-2.9). This segment averages about 15 feet deep and 250 feet wide. Temperatures were relatively constant along the length of Segment 2 but some horizontal stratification did exist. The temperatures are affected by lake intrusion but not to the same extent as the turning basin. Outfall 002 discharges to this portion of the river and heated river water enters from upstream.

The Black River turning basin (RM 2.9-2.4) is the third segment. The turning basin is dredged periodically by the U. S. Army Corps of Engineers to a depth of about 30 feet and averages about 600 feet wide. Large quantities of water flow upstream from the lake and mix with the heated water discharged from Outfalls 003 and 004 and the heated water entering from upstream. Intake WI-2, located in Segment 3, supplies the water discharged at Outfalls 002, 003, and 004. Temperatures were relatively uniform across the surface; however, vertical temperature stratification existed throughout the basin during the July 1974 survey.

MATHEMATICAL MODEL

Each of the segments described above was analyzed separately to determine the allowable thermal loads which can be discharged to the river. Daily steady-state conditions were assumed throughout the analysis. This assumption proves reasonable for the Black River because diurnal variations of the flows, heat loads and upstream river temperature were not significant. Complete mixing of the heated discharge with the receiving water was also assumed. The large discharge flow at Outfall 001 in relation to the upstream river flow results in complete mixing just below the outfall. Large discharge flows at Outfalls 002, 003, and 004 resulted in a relatively constant horizontal temperature distribution a short distance from the respective outfalls. Complete vertical mixing was also assumed despite vertical temperature stratification that occurred during the July survey in Segments 2 and 3. This assumption affects only the surface heat exchange term in the energy budget. Based upon the July 1974 data, this assumption introduces an error of less than 1% to the temperature computations.

The Edinger and Geyer one-dimensional formulation (1) was applied to Segment 1. The formulation is based upon the concept that a raised temperature resulting from a heated discharge will approach the natural stream temperature by the exchange of heat at the air-water interface. Assuming the heat added to the water body to be thoroughly mixed, the rate at which the temperature changes in the downstream direction is considered proportional to the product of an exchange coefficient and the temperature excess. Under steady-state conditions the equation used for estimating temperature downstream of a heated discharge is:

$$T = E + (T_m - E)e^{-\left(\frac{KA}{\rho C_p Q_R}\right)} \tag{2}$$

Where:

Q_R = river flow rate ft^2/day

TABLE 1

Average Computed Intrusion Flow (cfs)

Station	River Mile	Lake Concentration (1)	Bottom Concentration (2)
7	3.88	45	69
6	3.35	95	194
5	2.85	127	192
4	2.40	510	1342

(1) Intrusion flow was computed by setting the concentration of sodium and chloride in the intrusion flow equal to the measured values in the lake.

(2) Intrusion flow was computed by setting the concentration of sodium and chloride in the intrusion flow equal to the measured value at the bottom of the next downstream station.

E = equilibrium temperature, °F

K = exchange coefficient, BTU/ft^2-°F-day

A = surface area of the stream to the point where T is determined, ft^2

= density of water, 62.4 lbs/ft

C_p = heat capacity of water, 1 BTU/lb-°F

T_m = mixed temperature of the stream and the heated effluent at the outfall

The equilibrium temperature (E) used in Equation 2 is defined as the temperature at which the net exchange of heat at the air water interface is zero.

A different formulation was employed for Segments 2 and 3. The low stream velocities and the uniform surface temperature distributions of these two segments indicate that a cooling pond formulation would more accurately represent actual conditions. In this formulation, a heat budget equation was constructed. Under steady-state conditions the total heat content of the segment remains constant and the heat budget equation can be solved for the cooling pond temperature.

The heat budget which applies to both segments is:

$$H_O+H_U+H_L-H_I-H_D-H_S = 0 \qquad (3)$$

Where:

H_O = heat added at the outfalls

H_I = heat removed by the intakes

H_U = heat entering at the upstream end of the reach

H_L = heat entering from lake intrusion flow

H_D = heat leaving at lower end of the reach

H_S = heat lost at the water surface

The expression used to estimate the surface heat exchange, H_S is:

$$H_S = KA\ (T_S-E) \qquad (4)$$

with T_S being the water surface temperature and the other variables are as defined previously.

All heat terms except H_S in Equation 3 represent advective heat transfer resulting from the transport of water into or out of the segment. The heat contained in the flowing water is given by the general expression:

$$H = \rho C_p Q T \qquad (5)$$

In the analysis of Segment 2, H_O in Equation 3 is the heat added at Outfall 002. There are no industrial water intakes in Segment 2 therefore H_I is zero. Substituting Equation 4 as well as the appropriate advective heat transfer terms into Equation 3 and solving for the Segment 2 temperature results in the following:

$$T_{S2} = \frac{\rho C_p(Q_U T_U+Q_2 T_2+Q_L T_L)}{KA+\rho C_p(Q_L+Q_2+Q_U)} + KAE \qquad (6)$$

Subscripts denote where the water came from prior to complete mixing in Segment 2 (i.e. upstream, U; Outfall 002,2; lake intrusion, L).

A similar analysis was used to derive the temperature equation for Segment 3, the turning basin. Process water at the basin temperature is withdrawn at intake WI-2 and discharged at Outfalls 002, 003, and 004. Substituting Equation 4 and the advective heat terms into Equation 3 and solving for the basin temperature yields the expression:

$$T_{S3} = \frac{\rho C_p\left[(Q_U+Q_2+Q_L)T_{S2}+Q_3T_3+Q_4T_4+(Q_{LB}-Q_L)T_L\right]+}{KA+\rho C_p(Q_U+Q_2+Q_3+Q_4+Q_{LB})} + KAE \qquad (7)$$

Where:

Q_{LB} = lake flow entering the basin at the downstream end, cfs

Q_L = lake water flowing upstream along the bottom to the mid-section, cfs

The above equation takes into account that not all lake intrusion water entering the basin is mixed within this section. A portion, Q_L, flows upstream to Segment 2.

VERIFICATION

Before Equations 2, 6, and 7 were used to determine allowable thermal loads at the water quality design flow of the river, the models were tested on the Black River using July data with the resulting computed temperatures compared to measured values. The July data base provided an excellent test for the thermal models because the average measured flow upstream of U. S. Steel (22.6 cfs) was very close to the water quality design flow for the river (21 cfs), and U. S. Steel was at maximum production.

For the July verification, the equilibrium temperature (E) for all segments was set equal to the flow weighted average of the values measured at French Creek and Station 10 because there are no significant thermal discharges upstream of U. S. Steel. In addition, equilibrium temperatures computed using procedures outlined in Reference 2 and average daily meteorological conditions recorded at Cleveland, Ohio, agreed very well with the assumed values. The value for the exchange coefficient (K) was obtained from the report "Effects of Geographical Location as Cooling Pond Requirements and Performance"(2).

For computing Segment 1 temperatures, Equation 2 was applied first from Outfall 001 to Outfall 005 (RM 5.0-3.92) and then from Outfall 005 to intake WI-3 (RM 3.92-3.88). Mixed river temperatures (Tm) at Outfalls 001 and 005 were calculated from measured effluent temperature and computed river temperatures immediately upstream of the outfalls. The three-day average computed temperature along with the maximum minimum and average measured temperatures are shown in Figure 3.

Segment 2 temperatures were computed on a daily basis, the same period for which the lake intrusion flows were determined. In applying Equation 6 to the Black River the lake intrusion flow computed at Station 6 using Station 5 bottom concentration was used. Correspondingly, the temperature measured at the bottom of survey Station 5 was used as the intrusion water temperature. Station 6 intrusion flow was chosen instead of that determined at Station 5 because Station 6 is located close to the center of Segment 2 and flows there would more likely represent the average intrusion flow throughout the segment. Daily average temperatures recorded at Station 7 and for Outfall 002 were also input to Equation 6. The average of the three daily values is plotted in Figure 3.

Black River turning basin temperatures were computed daily using Equation 7. Lake intrusion flows calculated with lake concentrations of sodium and chloride were used in the computations since flows computed with bottom concentrations appeared unreasonably high. Daily average temperatures and flows measured at Outfalls 003 and 004 were input to Equation 7. The average of the top, middle, and bottom temperatures measured at Station 6 was considered representative of the upstream water temperature entering the basin. The average computed basin temperature is presented in Figure 3.

The computed temperatures along the entire river agree well with the measured values, Figure 3. In Segment 1, computed temperatures are generally within the range of measured values recorded at each station located within the segment. Average computed values at the lower end of the segment (RM 3.88) agree within 1°F of average value measured at Intake WI-3. The computed Segment 2 temperature was also within 1°F of the average temperature measured at Station 6 mid-depth. Computed Segment 3 temperatures agree well with average measured temperatures throughout the basin. The calculated value is about 3°F above the total average temperature measured throughout the basin and about 2°F below the average temperature recorded in the top 9 feet of the basin where most of the heat is discharged. This result was expected in that a portion of the cool lake water was not mixing with water in the basin but instead was flowing upstream and mixing in Segment 2.

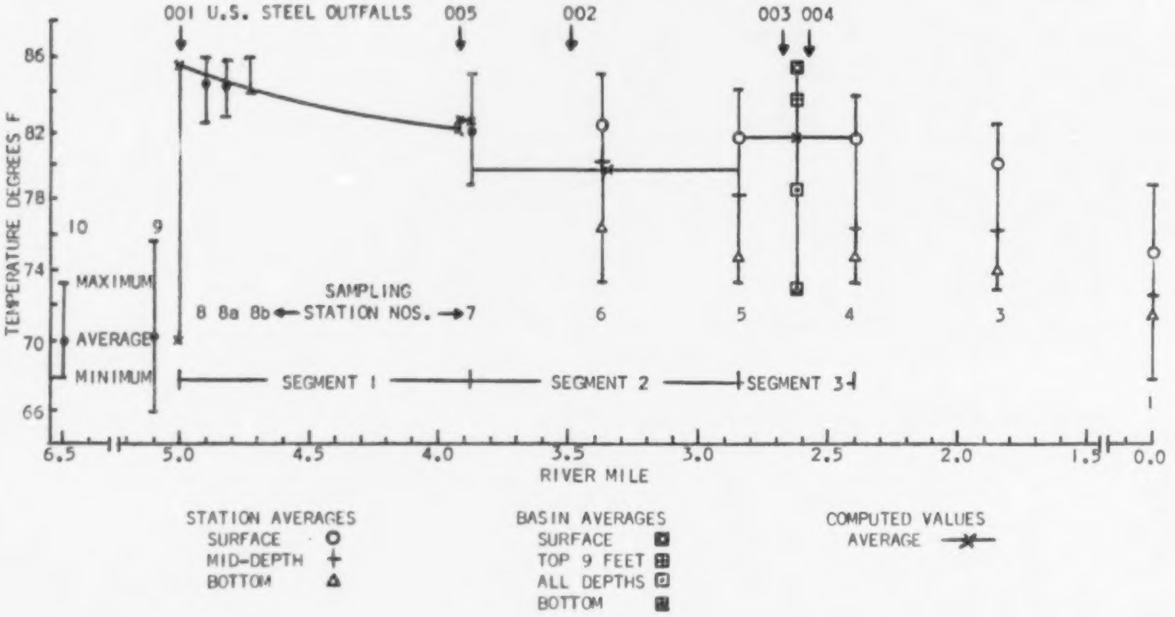
Based upon the ability of the computational procedures to replicate measured temperatures during low flow conditions within reasonable limits, the equations developed in the previous section were employed to compute allowable thermal loads from the U. S. Steel Lorain Works.

PROPOSED THERMAL LOADINGS

In computing allowable thermal loads, the mixed river temperature in the segments were set equal to the natural river temperature plus the maximum temperature increase permitted in the water quality standards, 5°F. The discharge temperatures and the associated heat loads were then determined using the equations developed and verified above. The water quality design flow of the river upstream of U. S. Steel was assumed in the computations (21 cfs). To simplify the analysis the temperature of the river upstream of U. S. Steel, the lake temperature and the equilibrium temperature were set equal. This assumption is reasonable in that there are no significant heat discharges above U. S. Steel. The natural water temperature used in the analysis was obtained from Reference 2 and is based upon average meteorological conditions recorded at Cleveland, Ohio during September, the month when low flows generally occur. The exact equilibrium temperature is relatively insignificant in computing the temperature profile due to the fact that the water quality standards are based upon increases above natural temperature and maximum temperatures are currently not exceeded with existing loads.

To compute the proposed heat loads at Outfall 001, the allowable temperature increase from Intake WI-3 to Outfall 001 was determined. This was achieved by first determining the discharge temperature which would increase the mixed river temperature at the outfall by 5°F and then simulating river temperatures down to Intake WI-3, using Equation 2. At Outfall 005 the maximum daily heat load discharged to the river was assumed to be 15 x 10^6 BTU/hour, slightly greater than the maximum value recorded during the July survey, 14 x 10^6 BTU/hour. The computed temperature and the river flow at Intake WI-3 were assumed to mix with the average daily lake intrusion flow at the intake. Intrusion water temperature was assumed equal to the lake temperature, therefore allowing the maximum heat load to be determined. The results indicate that a

FIGURE 3
BLACK RIVER TEMPERATURE VERIFICATION



temperature increase of 3.4°F may be imparted to the flow discharged at Outfall 001. Using the following equation the allowable heat load at 001 was determined to be 58 million BTUs per hour.

$$H = \rho C_p Q_1 \Delta T_1 \tag{8}$$

Where:

Q_1 = flow discharged at Outfall 001, cfs

ΔT_1 = allowable discharge temperature increase above the intake temperature, °F

Equation 6 was used to determine the allowable thermal loads discharged at Outfall 002. Setting the temperature of Segment 2 to 5°F above natural temperature, Equation 6 was solved for the temperature at Outfall 002. The intrusion flow determined assuming lake concentration was used in the computation to be consistent with the assumption that the intruding water was at lake temperature. The results indicate that Outfall 002 can discharge at a temperature 16.9°F above equilibrium temperature. Assuming the water withdrawn from the basin at Intake WI-2 to be 5°F above equilibrium, Outfall 002 can discharge at a temperature 11.9°F above the intake value or using Equation 8, 123 million BTUs per hour.

A similar procedure was used to determine the combined thermal load discharged from Outfalls 003 and 004 into the turning basin. The average temperature of the turning basin was set equal to 5°F above equilibrium and Equation 7 was solved for the net heat discharged to Outfalls 003 and 004. Lake intrusion flow was assumed equal to the average daily value determined using lake concentrations with the intrusion temperature at equal to the lake temperature. The flow entering from upstream, which was composed of lake flow, the flow from Outfall 002, French Creek, and the river above U. S. Steel was assumed to be 5°F above equilibrium as set in the previous computation. The combined heat load for Outfalls 003 and 004 was determined to be 515 BTUs per hour. This corresponds to a ΔT of about 16°F for the total flow of Outfalls 003 and 004.

Prior to the July 1974 survey, the Government had estimated thermal loadings from U. S. Steel to be acceptable in terms of achieving the 5°F ΔT standards. These loadings were proposed as effluent limitations pursuant to settlement of Civil Action C71-445 (N.D. Ohio) against U. S. Steel (Table 2).

Equations 6 and 7 were employed to determine the resultant temperature of Segments 2 and 3 using the proposed settlement loadings. All other inputs and flows were kept the same. Segment 2 temperature, computed assuming a thermal load of 67 million BTUs per hour at Outfall 002, was found to be 3.7°F above the ambient stream temperature. With this computed temperature and 600 million BTUs per hour from Outfall 003 and 004, Segment 3 was computed to be 5.3°F above ambient. An allowable thermal loading of 600 million BTUs per hour from Outfalls 003 and 004 appears reasonable considering the sensitivity of the basin temperature to lake intrusion flow, and the uncertainty involved in estimating intrusion flow. Reduction of thermal loads to 600 million BTUs per hour can be accomplished without substantial additional capital expenditures whereas reduction below that value will require costly additional cooling towers.

TABLE 2

U. S. STEEL LORAIN WORKS THERMAL LOADINGS

(10^6 BTU/hr)

Outfall	July 1974 Discharge	Loadings from this Analysis	Proposed Settlement Civil Action C71-445
001	177	58	60
005	13	15	10
002	303	123	67
003,004	694	515	600
Total	1187	711	737

Based upon this analysis, Ohio Water Quality Standards for temperature can be maintained on the Black River by reducing U. S. Steel Lorain Works heat loadings to the values presented herein or those proposed for settlement of Civil Action C71-445.

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WATER MODELING IN OHIO EPA

Robert G. Duffy
Water Quality Surveillance Section Chief
Ohio EPA
Columbus, Ohio

A. Ben Clymer
Consulting Engineer
Columbus, Ohio

Steady-State Stream Modeling in Ohio

Earliest Modeling Efforts

In 1965 the Ohio Department of Health developed the Garrett-McAnaney computer program for modeling steady-state stream quality for a river mainstem. The equations comprising the model were the Streeter-Phelps equations plus the equations for mixing at a node point. That is, the only parameters modeled were dissolved oxygen and BOD.

In 1972-73 the Ohio EPA developed the Clymer-Duffy computer program which enables a designer to determine various combinations of allowable loads from a single sewage treatment plant, such that water quality standards would not be violated anywhere downstream.

Features of the Garrett-Clymer-Duffy Models

Two advanced stream water quality models were developed by Ohio EPA in 1973 to project allowable loads for non-conservative parameters (i.e. D.O., BOD_5, NH_3-N). The two models were a "mainstem" model and a "mini-basin" model. The equations used in both models were obtained by closed-form integration of the linear constant-coefficient differential equations for first order kinetics. Mixing equations were written at each node point.

A feature unique to the mini-basin model is a set of equations to calculate the average stream velocity and depth when cross-section data are unavailable. These equations are based on the Chezy-Manning formula for channel flow.

In the mainstem model the change in D.O. as water flows over a dam is taken into account. The reaeration equation over a dam is described by Klein (1). The mainstem model allows for the borrowing of water from a river for once-through cooling purposes. A reduction in D.O. concentration is calculated, if the water is heated beyond saturation. A special canal subroutine was developed for the Cuyahoga River whereby a certain volume of water is diverted from the river to a canal running parallel to the river. Overflows from the canal divert water back into the river at several points. Phenol and cyanide decay, and hydrolysis of organic nitrogen to ammonia is also modeled in the mainstem model.

The effect of benthal deposits on D.O. is addressed in both models. All suspended solids are assumed to settle out behind a dam pool or elsewhere only if the stream velocity is less than 0.6 ft./sec.

Osman-Clymer-Kim Model and Program

The Garrett-Clymer-Duffy programs lacked some features which became desirable in 1975 in connection with a multibasin planning project, denoted herein as the Water Quality Planning Model Project, or "WQPM Project". These desired features were:

1. Ability to model a branching configuration of tributaries along with a mainstem, instead of just one chain of reaches;
2. Inclusion of algebraic formulas for the costs of waste-treatment and waste-conveying facilities;
3. Provision of an automatic load-allocation "loop" to insure that dissolved oxygen would meet water quality standards everywhere;
4. Addition of models for certain nonconservative parameters, such as the count of bacteria per unit volume;
5. Consideration of time of travel as a given value for each reach, from which velocity would be calculated as reach length divided by time of travel;
6. Provision for conservative substances as parameters;
7. Incorporation of a pre-existing in-house stream temperature program as a subroutine in the WQPM program;
8. Refinement of the formula for the oxidation rate "constant" for phenol to incorporate non-linear dependence upon temperature and concentration;
9. Inclusion of pH as a known input for each reach.

In all other respects the WQPM builds upon the Garrett-Clymer-Duffy mainstem model.

Validation Check of Ohio EPA Model

The Garrett-Clymer-Duffy mainstem model output was checked against field data collected by the U.S.E.P.A. Michigan-Ohio District Office on Feb. 12-13, 1975. The comparison for dissolved oxygen (D.O.) is shown in Fig. 1. Fig. 2 compares D.O. field data collected by Ohio EPA in the Scioto River in August 1974. In both cases the difference is of the order of 1 ppm of D.O., which is typical for water quality models (2).

Past Applications

An early version of the Garrett-Clymer-Duffy mainstem model was applied to the Little Miami River. This model was unable to simulate reaeration over a dam, benthal demand, or thermal withdrawals. However, the model applied to the Scioto, Mahoning, and Cuyahoga Rivers did simulate these phenomena. When modeling the Cuyahoga River, the canal subroutine was used. The mini-basin model was applied to problem areas in the Maumee, Hocking, Rocky Fork, Licking and Wabash Basins, including Findlay, Lima, Lancaster, Mansfield, and Newark. All of the foregoing studies constitute the modeling work that has been done to date by this agency to comply with the requirements of Section 303(e) basin planning studies.

Present Applications

The WQPM project is scheduled to prepare and analyze long-range wastewater treatment plans for major portions of the following basins by September, 1976: Little Miami River, Great Miami River, Mad River, Stillwater River, Alum Creek, Darby Creek, Tuscarawas River, Chippewa Creek, Sandy Creek, and Nimishillen Creek. These ten segments include representatives of most of the water quality problems which occur in Ohio.

The studies being performed have been designed to make maximum use of the Ohio EPA Water Quality Planning Model. Appropriate regionalization and economical processes for all new treatment plants will be found which will meet all present water quality standards until the year 2000.

Near Future Applications

The "Title X" project will utilize models developed by Ohio EPA to assess the impact of point source discharges in the Scioto, Muskingum, and Little Beaver Creek Basins. Cost-benefit assessment of different waste treatment schemes, including regional waste treatment plants, is planned. Plans are being formulated to model the impact on water quality of a 1" rainfall following a prolonged dry period. Modeling of conservative and non-conservative elements to insure compliance with water quality standards will be emphasized in the Title X program.

Another application of the models will be made by the Water Quality Standards Section of the Ohio EPA for the purpose of revising water quality standards.

Presumably these models will find application also in future Section 303(e) basin studies and 208 studies.

Limitations of the Stream Water Quality Models

All models mentioned thus far have definite limitations, which prevent them from being useful for some purposes of the Ohio EPA:

1. These existing models assume steady flow, which is an invalid assumption for the study of urban or rural runoff from a storm, or any other transient flow problem;

2. The models assume one-dimensional flow, which is not applicable to a wide and/or stratified reservoir or estuary;

3. The programs are not designed to be economical tools for Monte Carlo studies of the stochastic effects of stream flow, sewage treatment plant performance, influent flow and composition, etc., upon stream water quality;

4. Because instantaneous and perfect mixing are assumed at each node point throughout the cross-section, the models cannot evaluate water quality distribution in a mixing zone;

5. Since models fail to treat the biota explicitly (except for Coliforms), they cannot be used to draw conclusions about the ecosystem in a stream;

6. The programs do not relieve the user of all tedious tasks in connection with the preparation of input data; hence, additional labor-saving features might be desirable;

7. The models do not deal with a thermal plume in a river or lake.

Accordingly, there is clear need for research and development of other types of model, as discussed further below.

Research and Models Needed

Unsteady Stream Flow and Water Quality Model

The appropriate equations for transient (unsteady) stream velocity, depth, and concentrations of a pollutant having first-order kinetics are:

$$(1)\quad -\frac{\partial U}{\partial t} = g\tan\alpha + g\frac{\partial H}{\partial x} + U\frac{\partial U}{\partial x} + \frac{3\mu}{\rho H^2}U + \frac{g}{2}\frac{H}{W}\frac{\partial W}{\partial x}$$

$$(2)\quad -\frac{\partial H}{\partial t} = \frac{1}{W}\frac{\partial Q}{\partial x}$$

$$(3)\quad Q = WHU$$

$$(4)\quad \frac{\partial c}{\partial t} = \frac{c}{W^2}\frac{dW}{dH}\frac{\partial Q}{\partial x} - U\frac{\partial c}{\partial x} + \frac{1}{HW}\frac{\partial}{\partial x}\left(KHW\frac{\partial c}{\partial x}\right) - K_1 c + F(x,t)$$

$$(5)\quad W = W(H,x)$$

where U is section-average velocity, t is time, g is the acceleration of gravity, tan α is the slope of the stream bed (+ up), H is section-average depth, x is the space independent variable along the stream centerline, μ is equivalent viscosity, ρ is water density, W is section width, Q is stream flow rate, c is pollutant concentration, K is the longitudinal diffusion coefficient, K_1 is the kinetic rate constant of "decay" of c, and F (x,t) is a varying and distributed source. The partial differential equations (1, 2,4) can be converted to ordinary differential equations by spatial finite differencing of the dependent variables. They can then be solved by numerical integration in time.

The desired model should have the following features:

1. Ability to model depositing and resuspending of at least one size-and-density class of suspended solids;

2. Inclusion of nitrate and at least one form of phosphorus from rural runoff as parameters;

3. A lumped model of any sewer system and treatment plant in the area;

4. Inclusion of urban and/or rural runoff during and shortly after a storm.

Reservoir and Lake Models

Ohio has numerous reservoirs and lakes in which water quality is of concern. Ohio also has many rivers which discharge into Lake Erie. It is desirable, therefore, that the Ohio EPA have computer programs capable of modeling pollution, photosynthesis, wind-driven currents, etc., in a lake well enough for water quality management purposes.

The simplest case of a reservoir is one which results from a dammed up stream and which is relatively narrow. When the water is not stratified, it can be modeled as a deep stream. When the water is stratified, it might be dealt with as two streams, one on top of the other, with a minor amount of mutual coupling. However, most reservoirs and lakes are so wide that the mixed-stream assumption would be invalid, necessitating a treatment in at least two dimensions (lateral and longitudinal). A wide dam pool in a stream should be modeled as a lake, especially if it is used as a source of cooling water.

The parameters of lake models which are most important include the velocity and temperature fields, D.O., BOD, benthic demand, and nutrients. Most of the problems can be considered in seasonal steady-state, although some are progressive during a season, as in the case of a lake bottom going anaerobic in summer as a result of organic matter.

There seem to be available a number of models meeting most of the foregoing requirements. (3-5)

"Estuary" Models

The rivers in Ohio which flow north have "estuaries" where they enter Lake Erie. In an estuary there are changing gradients of temperature and concentrations of salts. A city with substantial industrial and municipal discharges to an estuary might require special water quality standards. An estuary model is needed for this purpose.

Many phenomena complicate the modeling of such an estuary (6): a thermocline at some times of year, currents and circulations due to the wind vector, a wedge of cold water at the bottom from lake or river, and sloshing back and forth of water (at much greater flow rates than the river flow) due to lake level fluctuations. These problems are at the frontier of the modeling art. However, simpler estuary models are available. (7-9)

Stochastic Stream Model

Recognition of the essentially-stochastic nature of water quality is implied in the practice of expressing standards in terms of 7-day 10-year low flow. It would be desirable to push the stochastic approach to water quality further by development and use of a stochastic model of stream minimum D.O. resulting from rainfall episodes. Because of the cost of the large number of long computer runs, it is not economically feasible to enclose a transient stream segment, sewer system, and treatment plant model in a Monte Carlo (repeated trials) loop. Accordingly, it is necessary to shorten the time for each iteration run. One approach is to replace the transient model with a nonlinear algebraic stochastic model containing the principal phenomena, component frequency distribution and other building blocks.

One way to get the algebraic model is to do regression analysis on the results from a transient model in a variety of cases. A complementary way is to assemble the stochastic model from theoretical building blocks, which include empirical parameters having unknown values to be determined from model-fitting studies with the transient model.

Mixing Zone Models

Many water quality standards are expressed in terms of a mixing zone downstream of a discharge. However, stream models have customarily been based upon the assumption of instantaneous uniform mixing across the entire cross-section at the discharge. Thus there is need for a two-dimensional model capable of describing the steady-state plan view concentration field in the mixing zone. The required inputs are the stream flow, width, average depth, bottom roughness, characteristic height or other determinant of transverse diffusion (10), and discharge parameters (flow, concentration, location, and direction of discharge). Ideal vertical mixing would be assumed in shallow streams.

Biochemical Kinetics Models

There is much to be learned about the empirical functions which describe the rate constants of biochemical "decay" of pollutants in a stream. One of us (A.B.C.) has studied the rate constant for the oxidation of phenol as a function of temperature and concentration. The data base used was for the 3-mile reach on the Mahoning River from Struthers to Lowellville. At both ends of this reach the Ohio EPA had determined phenol concentration and temperature 30 times from 1973 to 1975.

The usual practice of making the logarithm of the rate constant linear in the temperature was found to be grossly inadequate by not showing a peak; a quadratic term is necessary, and a cubic term is desirable. The logarithm of the rate constant should contain also a term proportional to the logarithm of concentration. It is hoped that similar regression studies of the rate constants of this and other reactions will be performed in Ohio EPA and elsewhere.

Due to the poor reproducibility of the BOD_5 test, an in-house research project was initiated to determine if more reliable tests such as COD, TOC, or TOD could be used to model or estimate BOD_5. The carbonaceous component of BOD was studied by using a chemical to inhibit the nitrogenous component. Analysis of the data is incomplete, but preliminary results indicate that a strong correlation between BOD_5 & COD, BOD_5 & TOC and BOD_5 & TOD does not exist.

Stream Hydrology Models

Ohio water quality standards are expressed in terms of the 7-day 10-year critical low flow. However, the stream hydrological data are available ordinarily only at much higher flow conditions. It is necessary, therefore, to find a means to extrapolate the hydrologic data to critical low flow from the flow value which existed. Thus a model of stream hydrologic parameters as functions of flow is required.

The most commonly used model for this purpose is a power function, namely,

$$W = aQ^b;\ H = cQ^f;\ U = kQ^m$$

where the lower case letters are empirical constants.

The exponents must satisfy the constraint $b+f+m=1$, in order that the empirical formulas yield values of W, H, and U, whose product WHU equals Q. Points (b, f, m) can be plotted in an equilateral triangle as shown in Figure 4. The points representing the exponents for different cross-sections of a given stream tend to cluster or form a streak in the triangle. Thus the triangular plot is useful in studying data for the exponents.

Other Models

Ohio streams and lakes constitute ecosystems which are important to the Ohio EPA. The importance arises from, for example, the commercial and sports fisheries, on the one hand, and the difficulties associated with eutrophication and algae, on the other hand. However, the Ohio EPA has not yet done any aquatic ecosystem simulations. Nevertheless, as modeling evolves in the agency, such studies will be done in the next few years. Good progress in the development of freshwater ecosystem models has been made by the Deciduous Forest Biome project in the International Biological Program.

A benthic community analysis for the Scioto Basin was undertaken by the aquatic biology staff of Ohio EPA. Their findings clearly demonstrate that a good correlation exists between species diversity and D.O. This is illustrated graphically in Figure 3.

Dr. F.S. Bagi of the Ohio EPA has been applying least-squares regression to actual cost data from Ohio waste treatment facilities and interceptor sewers, in order to build up a cost model for a complete drainage basin. A preliminary version of such a cost model is currently being added onto the WQPM program, in order that alternative treatment plans for a basin may be compared on a cost basis. It is expected that the basin cost model will reveal opportunities for savings through regionalization.

In the near future several alternative treatment processes will be costed, when a % removal of BOD is specified.

Many of the foregoing types of models would be useful for long-range planning of treatment facilities. In all such applications, a need exists for a preprogram to generate projections of future flows and loads from all industrial and municipal plants in the basin. The user would supply data such as assumed constant growth rates of familiar parameters like daily per capita water usage, BOD and ammonia production, industrial production, and population.

Conclusion

Progress has been made by the Ohio EPA in the development and utilization of water quality models and computer programs, as described herein. However, the problems facing this agency will require the development and application of various advanced models.

Acknowledgements

The authors wish to acknowledge generous help from George Garrett, Paul Flanigan, Ed Armstrong, Dr. Tom Birch, and Pat Abrams, all of the Ohio EPA, in providing information and data for this paper. We are indebted to George also for having conveyed to us over a period of years much of his deep concern for and some of his extensive knowledge of water quality problems.

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FIGURE 1

OEPA MODEL VERIFICATION DATA FOR MAHONING RIVER

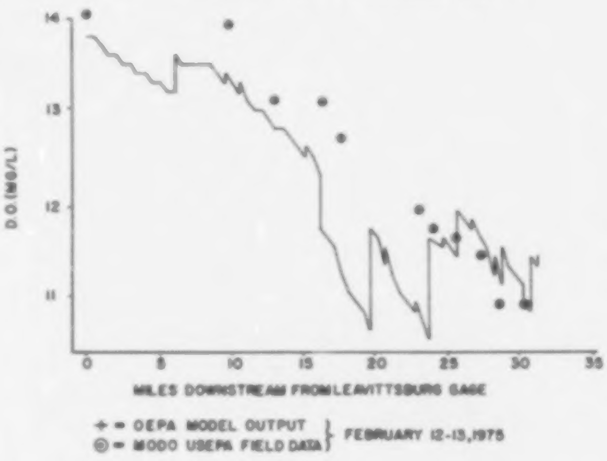


FIGURE 2

ACTUAL vs MODELED D.O. IN SCIOTO RIVER

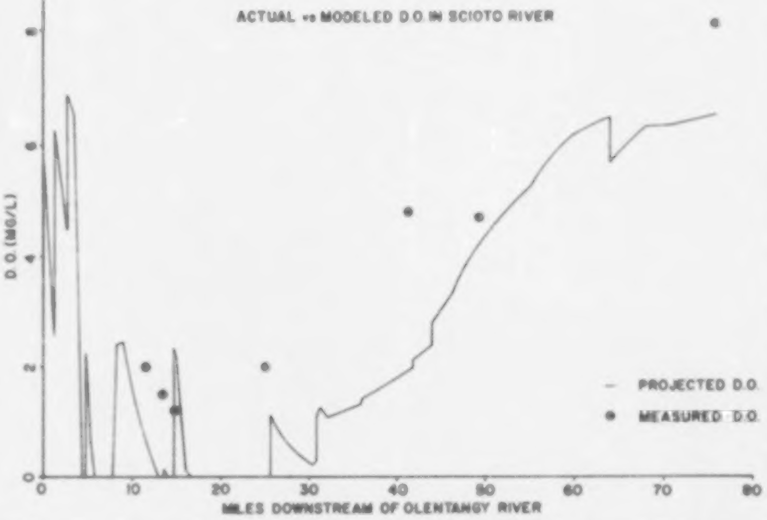


FIGURE 3

D.O. vs SPECIES DIVERSITY IN SCIOTO RIVER

FOR AUGUST, 1974

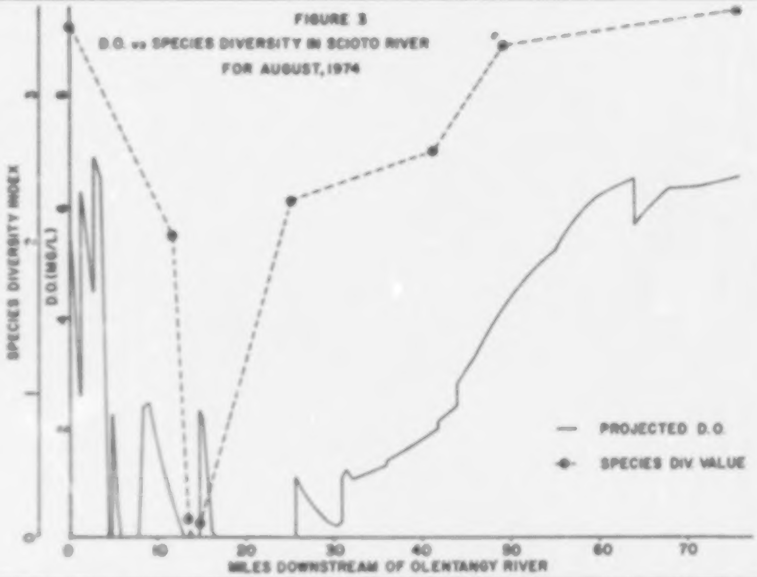
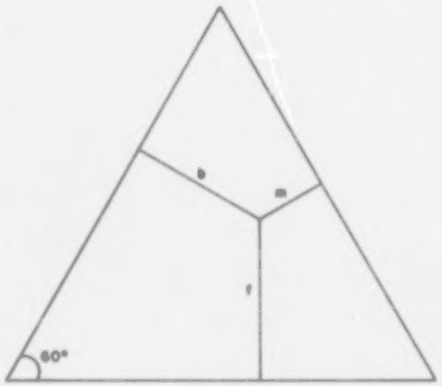


FIGURE 4

WATER MODELING IN OHIO EPA



THREE-DIMENSIONAL MODEL DEVELOPMENT FOR THERMAL POLLUTION STUDIES

Subrata Sengupta and Samuel Lee
School of Engineering, University of Miami
Coral Gables, Florida

and

Roy A. Bland
National Aeronautics and Space Administration
Kennedy Space Center, Florida

BACKGROUND

Because of the growing importance of thermal pollution and because of the possibility of detecting it by means of remote sensing, the National Aeronautics and Space Administration (NASA)-Kennedy Space Center (KSC) has sponsored a study on this many-faceted problem. A team of researchers at the University of Miami has been under KSC contract to develop a universally applicable three-dimensional thermal pollution math model. When completed this model will predict the three-dimensional motion and temperature of thermal plumes within waters to which they are discharged.

This mathematical model can include effects of winds, ocean currents, cyclic tidal flushings in bays and estuaries, variable winds and realistic bottom topography. Remotely sensed data and in situ measurements are used for model calibration and verification. An airborne scanner system backed up by satellite infrared remote sensing systems is used to measure water surface temperatures.

The airborne scanner system used is a Daedalus DS-1250 multispectral line scanner system and is installed in a C-45H Tri-Beechcraft (NASA-6). An Hg:CO:Te detector is used for sensing 8-14 micron IR radiation. The system is owned and operated by the NASA Kennedy Space Center. Two kinds of satellite data are used to supplement the aircraft-derived IR data. These are the NOAA-2 and NOAA-3 satellites, which operate in the 10.5 and 12.5 micron region with 0.5 nautical mile resolution. Also used in the study are data from the Air Force DMSP satellite, which operates in the 8-13 micron range with 0.3 nautical mile resolution.

This mathematical model will serve a dual purpose. It can be used in surveillance studies and also it will enable environmental planners to predict the behavior of hot discharges in a given region and, therefore, to determine whether such discharges exceed allowable temperature limits at depth and on the surface. In other words, this model can be used in the location of future nuclear power plants in order to select the most advantageous sites.

MATHEMATICAL MODEL DEVELOPMENT PLAN

After a feasibility study was completed in January 1974, it was concluded that the mathematical model development would take four years to complete. As an end product, the model will be well documented, readily transferable, and initial and boundary conditions easily altered so that the model can be universally applicable. This four-year period will be divided into four phases.

In the first phase, the basic concepts of the model were established and the optimum numerical scheme (finite differences) for the solution of the math model's governing equations was selected. In the second phase, completed in December 1975, the model was developed and applied to Biscayne Bay, Florida, using the Cutler Ridge power plant thermal discharges as a testing case. Both rigid lid and free surface models of Biscayne Bay were written during this phase, but only the rigid lid far field version has been completely verified to date. Velocity and temperature fields have been computed for different atmospheric conditions and for different boundary currents produced by tidal effects. The computations have been carried out for different time periods between one and six hours of real-time. Four aircraft infrared data runs, roughly one each quarter, were made over Biscayne Bay during this phase to supply data for the model.

In the third phase, which began in January 1976, a twelve-month period will be devoted to three tasks. The modeling of Biscayne Bay will be completed and computer results verified against remote sensing and in situ measurements. In the second task, the mathematical model will be revised as needed and applied to the St. Lucie, Florida, nuclear power plant, which discharges onto the off-shore continental shelf. This will be an interesting contrast to Biscayne Bay, which is a shallow lagoonal estuary. The third major task results from a recommendation by several EPA and NRC/ERDA officials. Their recommendation was to initially apply the rigid lid version of the model to a deep lake reservoir. In consultation with the progressive Duke Power Company, it was concluded that the rigid lid model should first be tested on a thoroughly understood lake where abundant real-time measurements are taken. The lake selected and approved was Lake Belews, North Carolina, which serves as a cooling reservoir for a large fossil fuel plant. Thus, the third task in this phase of the implementation plan will be to model Lake Belews, North Carolina, in cooperation with and under the sponsorship of the Duke Power Company.

In the fourth and final phase of the development plan, the mathematical model will be further generalized so that it will be readily applicable to any geographical discharge area site. The computer program will be finally documented so as to afford a user computing facility minimum difficulty in making this program operational. In cooperation with EPA and NRC/ERDA officials as well as the electrical power generating companies, the NASA-KSC will work toward utilizing this model as an industrial standard. As needed, further applications of the model will be carried out in this final stage.

MATHEMATICAL MODEL

A considerable amount of work has been done in modeling thermal discharges. A three-dimensional model including the effects of buoyancy, topography, and other parameters has not been developed yet. Akers[1] discussed some of the models that are in existence. Policastro[2,3,4] in a series of review papers has compared the existing plume models with field data. He considered a range of models from analytical to quasi-three-dimensional numerical models. Harleman's[5,6,7] pioneering work led to a numerical model with Stolzenbach,[6] which has been widely used in plume analysis. The only existing complete three-dimensional models are by Waldrop and Farmer[8] and Paul.[9] However, Paul's model assumes symmetry, thereby eliminating the possibility of including wind or current effects. Both models are for constant depth basins. The objective of the present study is to develop a comprehensive three-dimensional model including the effects mentioned above.

Details of formulation, solution, and development have been discussed in reports by Lee et al.[10,11] The need for remotely sensed data in model development and verification has been discussed by Sengupta et al.[12] A general description of the various models comprising the thermal pollution mathematical model package will be presented here.

Thermal anomalies caused by a heated discharge usually affect areas of a few miles in extent. Initially, the discharge is dominated by a jet-like behavior. Then, turbulent entrainment and buoyancy influences the trajectory and spreading. Finally, the flow is governed by the far field conditions and the ambient meteorological state. The domain of interest can be classified into a near field, where effects of the discharge are significant, and a far field, which affects the plume but is not appreciably affected by the plume. The numerical characteristics of these two domains are quite different. The procedure, therefore, is to obtain a far field solution with a coarse finite difference grid and to use this to obtain the near field (plume) solution using a finer mesh size.

The governing equations describing the state at a point in the flow field are a system of coupled, non-linear, second-order, three-dimensional partial differential equations which satisfy local conservation laws for total mass, species mass, momentum and energy. The constitutive equations complete the system of equations. In laminar flows the molecular transport properties for heat and mass transfer may be used. Most environmental situations are, however, turbulent. The time averaged transport equations are therefore used. The turbulent closure condition is specified by approximating the Reynolds stress terms by eddy transport coefficients. For studies where salinity variations are important, a salt conservation equation similar in form to the energy equation can be added.

The surface waves can be eliminated by imposing a rigid lid condition whereby the vertical velocity at the surface is equated to zero. The transients are somewhat distorted but the steady-state general circulation is not significantly affected. The elimination of surface gravity waves allows larger integration time steps, thereby reducing computation time. However, in cases where surface elevation changes are significant and transients are to be investigated, a free surface model has to be used. The rigid lid formulation for a variable depth basin has been developed by Sengupta and Lick.[13] A free surface model has been used by Freeman et al.[14] to study the circulation and periods of oscillation of Lake Huron.

The computer program package that is being developed is to be applied in a wide variety of geophysical situations, so both the free surface and rigid lid models are being developed. Both these models are further sepcialized to be applied to near and far fields. Therefore, there are four separate programs.

Rigid lid model

(i) Far field version

(ii) Near field version

Free surface model

(i) Far field version

(ii) Near field version

The rigid lid model has been used to obtain general circulation and temperature distributions in Biscayne Bay. The free surface model is in its final stages of development and application. The rigid lid model will be described here together with the results and the verification based on ground truth and remote sensing data. Figure 1 shows the program package with applicable geographical locations.

Rigid Lid Model

The programming difficulties for a three-dimensional basin suggest a stretching of the vertical coordinate with respect to the local depth. This converts the basin to constant depth. The same number of grid points in the vertical direction can be used at the shallow or deep parts of the basin without using variable grid sizes. The stretching introduces extra terms in the momentum equations. The details of the derivation are presented by Sengupta and Lick.[13]

The governing equations consist of the continuity equations, the three momentum equations, the energy equations, and the equation of state. The vertical momentum equation is simplified using the hydrostatic approximation. The Boussinesq approximation is made. Constant though different eddy transport coefficients are chosen for vertical and horizontal diffusion. The equation of state is an empirical relation between density and temperature. The vertical velocity at the lid is zero. This causes the surface pressure to be different from atmospheric pressure. The x and y momentum equations are integrated over depth and combined after differentiation with respect to x and y, respectively. The resulting Poisson equation is the predictive equation for surface pressure. The above set of equations with appropriate boundary and initial conditions constitute the mathematical model.

Initial and Boundary Conditions

The nature of the equations requires initial and boundary conditions to be specified. The velocities, temperature, and density are given throughout the domain as initial conditions. Boundary conditions are specified at the air-water interface, horizontal boundaries of the domain, the bottom of the basin and efflux points. At the air-water interface, wind stress and heat transfer coefficients are specified. The conditions on the lateral walls allow no slip and no normal velocity for the momentum equations. These walls are assumed to be adiabatic. At the floor of the basin, the conditions of no slip and no normal velocity are also applicable. The energy equation has a heat flux boundary condition, considered adiabatic for the present study. At points of efflux, the velocities are specified and the graident of temperature normal to the domain boundary is considered zero. These open boundary conditions are most difficult to specify.

Method of Solution

An explicit finite difference scheme is used to integrate the transport equation. The general finite difference form is:

$$\frac{u^{n+1}-u^{n}}{t} = (\text{convection})^{n} + (\text{pressure})^{n} + (\text{viscous})^{n-1,\ n,\ n+1}$$

Here u may be replaced by v or T (for the T equation the pressure term is not used). The spatial derivatives are centrally differenced using a modified Dufort-Frankel scheme to avoid time-splitting in long term integration. Its advantages have been demonstrated by Sengupta and Lick.[13] The pressure equation is approximated by a five-point scheme and solved by the Liebmann relaxation procedure. The algorithm is as follows:

a. Using values at time step n, calculate the forcing term for the pressure equation

b. Solve the pressure equation iteratively

c. Calculate u and v from the momentum equations

d. Calculate w from the continuity equation using u and v at n+1

e. Calculate T from the energy equation

f. Calculate ρ from the equation of state

The procedure is repeated for each time step.

APPLICATION AND VERIFICATION

Figure 2 shows a map of Biscayne Bay. The bay is open to the ocean on the eastern side through a shoal region and some creeks. The northern end is partially obstructed by a causeway. At the southern end a shallow region effectively separates the bay from Barnes Sound. There are two power plants located on the bay; one at Cutler Ridge and the other at Turkey Point. The far field conditions affect the thermal plume from the Cutler Ridge plant. The Turkey Point plant uses a cooling canal system.

The rigid lid model has been applied to Biscayne Bay. A wide range of meteorological conditions have been modeled and detailed results and evaluations presented in a report by Lee et al.[11] In this manner the program was calibrated and the parameters were chosen. For verification, the model results were compared with data gathered from a field experiment on April 15, 1975. NASA-6 thermal scanner runs were flown in the north-south direction. Ground truth data was used to correct for atmospheric effects and also to record the vertical variation of temperature in the bay. The average wind was from the southeast at 10 mph and the air temperature was 30°C. The tide was incoming. Figure 3 shows the interpolated isotherms drawn from the thermal IR data. There is a hot spot near Featherbed Banks. There are warm regions wherever the depth is shallow. Because the near shore regions are warmer, the central parts of basins of Card Sound are seen to have closer isotherms. There are warm spots near the group of islands at Caeser Creek and also near the island two miles south of Turkey Point. The verification for the model involved comparison of this thermal IR map with computed surface isotherms.

The numerically predicted circulation for the bay in the case described above is shown in Figure 4. The incoming tide is primarily diverted to the south. The effect of the wind is to turn the flow toward the northwest, though the tidal effect predominates. The current toward Rickenbacker Causeway is minimal. The velocities near the shoals are incoming. The mass flux through the creeks has very localized effects. The Featherbed Banks reduce the current magnitude, so the velocity increases in the deeper regions adjacent to the banks. The velocities also increase as the bay narrows to the south.

The measured quantities, namely wind speed (10 mph southeast), incoming tide, and ambient temperature (30°C), were used to obtain the temperature field. To minimize the effect of initial temperature conditions, the run was executed with as early a starting time as possible. At 9 AM near Cutler Ridge (I=11, J=3), the measured temperature was 25.6°C with no vertical stratification. Since this is a near shore location, the average temperature in the bay can be assumed to be lower. Since the detailed temperature field was not known as an initial condition, it was assumed that the bay was isothermal with a temperature of 24.5°C at 8 AM. The model predicted the conditions six hours later, which were compared with mid-afternoon in situ and remotely sensed data.

Figure 5 shows the surface isotherms predicted by the model. The surface isotherms show a hot spot over Featherbed Banks. The warmer near shore regions are quite clearly seen. The warm area near the islands in the southern part of the bay is also evident. The comparison with thermal IR data in Figure 3 is excellent. It should be noted that the IR data are not synoptic. There is a time lag of almost three hours between near shore flights and flights over the keys. Considering this time lag and the approximate specification of initial conditions, the model may be considered quite satisfactory for ecological studies.

The ground truth data were obtained only in the morning of the April 15, 1975, field experiment. Results for the model after three hours of heating can be compared with ground truth measurements at location I-11, J=7 at 11 AM. Figure 6 shows a transect of the bay along J=7. The predicted isotherms are shown, with ground truth data at locations marked by asterisks. It can be seen that the agreement is within 0.7°C. This is satisfactory for most environmental applications.

Conclusions

As part of a generalized model development program, a three-dimensional rigid lid model has been developed. Remote sensing and ground truth data have been used to calibrate and verify the model. The model has been found satisfactory in predicting the general circulation and temperature field in Biscayne Bay.

Acknowledgments

The authors wish to express their gratitude to Drs. N. Weinberg, H. Hiser, and Mr. James Byrne for their effort in processing the remote sensing and ground truth data. The effort of the NASA-KSC data analysis personnel and flight crews were an integral part of the investigation.

Figure 1. Application Chart for Numerical Models (University of Miami—NASA-KSC Project)

APPLICATION	THERMAL DISCHARGE				GENERAL CIRCULATION AND TEMPERATURE FIELDS			COASTAL BOUNDARY LAYERS		
MODEL	LAKE	RIVER	BAY	OCEAN	LAKE	BAY	OCEAN	LAKE	BAY	OCEAN
RIGID-LID NEAR FIELD MODEL	*	*	IGNORES LEVEL CHANGES					IGNORES LEVEL CHANGES	IGNORES LEVEL CHANGES	
FREE SURFACE NEAR FIELD MODEL	*	*	*	*				*	*	*
RIGID-LID FAR FIELD MODEL					*	IGNORES LEVEL CHANGES	IGNORES LEVEL CHANGES	*	IGNORES LEVEL CHANGES	
FREE SURFACE FAR FIELD MODEL					*	*	*	*	*	*

* Model Applicable

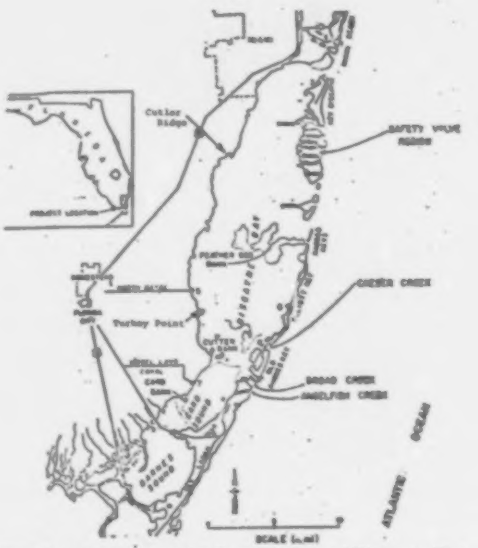


Figure 2. Map Showing the General Area of Biscayne Bay

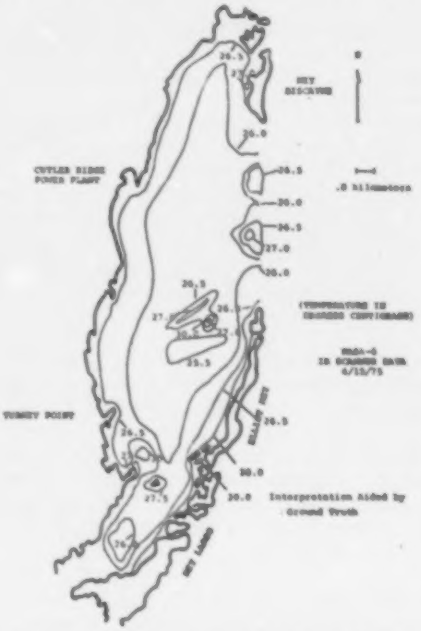


Figure 3. Biscayne Bay and Card Sound Florida

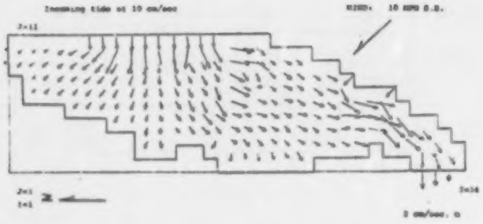

Incoming tide at 10 cm/sec
WIND: 10 MPH S.E.
J=11
J=1
I=1
I=34
5 cm/sec.

Figure 4. Surface Velocities

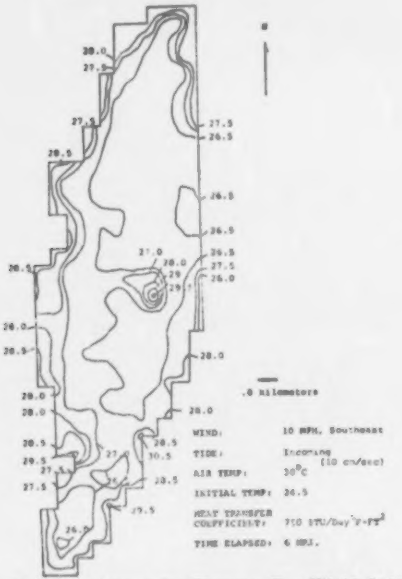

28.0
27.5
27.5
28.5
27.5
26.5
26.5
26.5
27.0
28.0
29
29
26.5
27.5
26.0
28.5
28.0
28.5
28.0
28.0
28.0
28.0
28.5
29.5
27.5
27
30.5
28.5
28.5
29.5
26.5
.8 kilometers
WIND: 10 MPH, Southeast
TIDE: Incoming (10 cm/sec)
AIR TEMP: 30°C
INITIAL TEMP: 24.5
HEAT TRANSFER COEFFICIENT: 750 BTU/Day °F-FT²
TIME ELAPSED: 6 HRS.

Figure 5. Surface Isotherms for Biscayne Bay (Rigid-Lid Model) (Temperature in Degrees Centigrade)

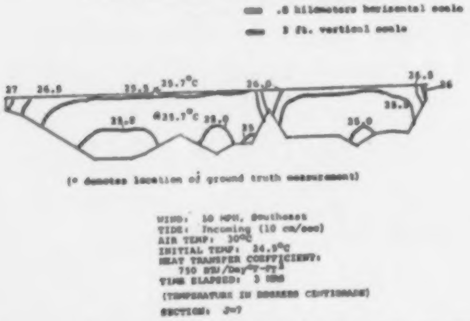

.8 kilometers horizontal scale
3 ft. vertical scale
27
26.5
25.5
25.7°C
26.0
25.5
26
25.0
25.7°C
25.0
25
25.5
25.0
(• denotes location of ground truth measurement)
WIND: 10 MPH, Southeast
TIDE: Incoming (10 cm/sec)
AIR TEMP: 30°C
INITIAL TEMP: 24.5°C
HEAT TRANSFER COEFFICIENT: 750 BTU/Day°F-FT²
TIME ELAPSED: 3 HRS
(TEMPERATURE IN DEGREES CENTIGRADE)
SECTION: J=7

Figure 6. Comparison of Calculated Isotherms for Vertical Section J-7 With Ground Truth Data

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SOME OBSERVATIONS ON MODELLING DISPERSION OF POLLUTANTS IN NEAR-SHORE WATERS OF LAKE MICHIGAN

Richard H. Snow
Engineering Advisor
IIT Research Institute
Chicago, Illinois 60616

ABSTRACT

Results of an investigation of the effect of effluents on water quality in the Calumet area of Lake Michigan are reviewed. The study showed that part of the effects could be directly traced to the plume of the largest effluent source, the Indiana Harbor Canal. Since the number of measurements in the plume was limited, modelling of the behavior of the plume was useful to show that the measured conditions were typical, and could be expected to occur during a large part of the time.

However, focussing attention on the plume ignored the more general pollution of near-shore water, which in one other Great Lakes location was shown to have a residence time of 40 days. The only existing model of the long-term dispersion of this pollution does not take into account the known and suspected behavior of the near-shore water movement. It is recommended that measurements of the behavior of the near-shore water be carried out to form the basis for dispersion modelling.

INTRODUCTION

It has long been noticed that the near-shore waters of the Calumet area of Lake Michigan contain higher concentrations of pollutants such as NH3-N and phosphorus than other areas of the Lake which are farther from large population centers.[2] The Calumet region is in the southwestern portion of the Lake, extending from Chicago to Burns Harbor, Indiana. Measurements of the water quality at various water intakes could not be directly correlated with known effluents, because the transport and dispersion of the water masses was not simultaneously measured or predicted.

A first step in understanding the effect of effluents on water quality is to correlate the measurements with the motions and dispersion of effluent plumes in the area. An attempt to do this was reported by Snow.[10] The effort met with some success and is briefly reviewed below. The purpose of the present paper is to discuss limitations in the approach based on the study of plume behavior, and to suggest an approach based on the movement of near-shore water masses covering a wider area and a longer time span than is observed in a plume.

STUDY OF IHC PLUME

The largest source of effluents in the Calumet region is the Indiana Harbor Canal (IHC). Figure 1 is a Skylab photo showing the IHC plume. In a recent study for the EPA[10] measurements of the water quality were correlated with motion and dispersion of the plume from the IHC over a distance of up to 19 km.

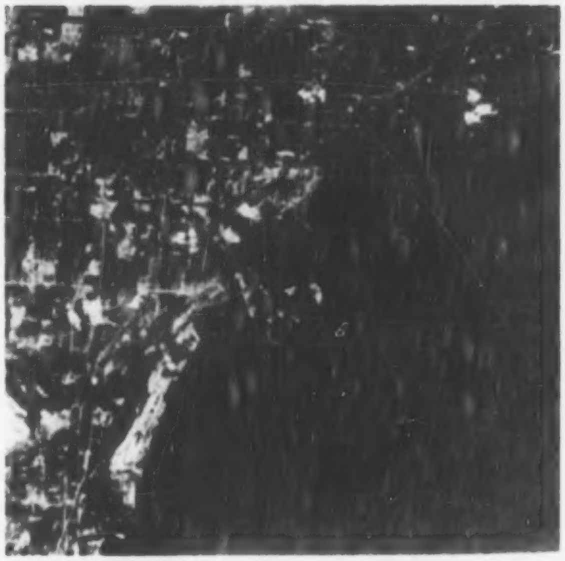

Figure 1

Skylab Photo of Calumet Area of Lake Michigan, Showing Plume From IHC, Sept. 13, 1973

The following parameters were measured, and this combination of measurements provided a fingerprint to identify and track the effluents from the IHC: NH3-N, total Fe, temperature, conductivity, chloride, fluoride, coliform bacteria, and others. Other agencies have measured such parameters as phenols, cyanide, oil, taste and odor, heavy metals, toxic bacteria and viruses.[10] Other pollutants may be expected, such as PCB's.

GRAVITY SPREADING AND MIXING

The water of the IHC is almost always warmer and less dense than the Lake water, and this gives rise to a typical estuary effect at the mouth of the Canal. The IHC is dredged to a depth of about 10 m; the warmer canal water flows out in the top 3-5 m of this depth, and colder Lake water intrudes in the bottom portion. This behavior is similar to that observed in a salt-water estuary, and described by Ippen.[4] The rate of gravity spreading is given by Parker and Krenkel[8] in terms of the wave velocity

$$U_\Delta = \sqrt{\frac{\Delta\rho}{\rho} gH} \qquad (1)$$

where

ρ is density of water, consistent units

g is acceleration of gravity, 9.80 m/sec^2

H is depth of heated water, m

Measurements of temperature and depth of heated water were taken at the mouth of IHC, Station CAL06, on three boat-sampling days, and are given in Table 1. Velocities were measured with a current meter, and density differences were computed from the measured temperature gradient. From these data and Equation 1 we can calculate the outflow velocity based on the spreading mechanism. It is compared with the measured outflow velocity in the last two columns of the table. The agreement is so good that this confirms the mechanism of outflow.

The colder Lake water which intrudes under the canal water mixes with the IHC water in the lower part of the canal. As a result of this inflow and mixing, the IHC water is already diluted 20 to 50% at the mouth of the canal, according to our measurements of inflow in Table 2 (Snow[10]).

Inflow is produced because the warmer canal water flows out of the harbor faster than it is supplied from upstream. The Lake water is drawn in to make up the deficit, and to conserve mass.

A calculation shows that gravity spreading is more important than inertial jet flow of effluents out of the IHC mouth. The ratio of these two effects is measured by the Froude number, F.

$$F = \frac{U_0}{\sqrt{\frac{\Delta\rho}{\rho} g H}} \qquad (2)$$

where

U_0 is centerline velocity of jet, m/sec

From data given in Table 1 we calculate F = 1.1. A value of F < 2 means that the gravity effect is more important than the inertia of the jet (Cederwall[3]).

Once the plume passes outside the mouth of the IHC, it continues to spread over the colder Lake water, just as oil spreads on water, because of the gravity difference. It seeks to flow out and become thinner, decreasing its gravitational potential. Such a wave-front is vertical and sharply defined (Cederwall[3]). Although the wave front is moving with respect to the bulk of the water, it may appear stationary if the water has the same velocity in the opposite direction. Parker and Krenkel[8] describe the phenomenon in some detail and review mathematical descriptions of it.

The behavior of the plume just outside the IHC mouth appears to depend on the interaction of gravity spreading with Lake currents that usually run parallel to the shore. This pattern is clearly shown by the Skylab photo, Figure 1. This photo suggests that there was a fairly strong general current in the main Lake water flowing from north to south, dragging the plume around the landfill. The plume gives the appearance of gravity-spreading behavior on the north boundary. The width of the plume is determined by competition between the spreading rate and the Lake current speed. The rate of spreading was predicted by a dimensionless correlation from the literature (Sharp[9]). The actual dilution factors were measured in the plume within a few km of the IHC mouth on 3 days. The model for spreading was used to show that the measured dilutions were typical, since the spreading depends on the known temperature difference and on the along-shore lake current speeds. The measurement

Table 1

GRAVITY FLOW AT IHC MOUTH (CAL06)

Date, 1973	Depth of outflowing layer, m	Temperature, °C		Density deficit, g/mℓ	Outflow velocity, m/sec	
		Top	Bottom		Calculated	Measured
November 14	3.5	15.9	10.0	0.00076	0.15	0.15
November 19	3.5	15.0	11.5	0.00045	0.12	0.13
December 7	3.5 5*	13.5	10.5	0.00034	0.10 0.12	0.13

*Depth of outflow was uncertain because a large eddy passed during one of two measurements.

Table 2

MEASURED FLOWS AT MOUTH OF IHC

Date	Total Outflow		Lake Inflow	
	m^3/sec	cfs	m^3/sec	cfs
November 14, 1973	89	3150	44	1546
November 19, 1973	102	3590	(14)	(495)
December 7, 1973	120	4226	(22)	(778)

of Lake currents is described below.

Temperature data from Storet indicate that the IHC is usually 5°C warmer than the Lake, and this is due to the fact that IHC water consists of Lake water that has been pumped through industrial processes and used for cooling. The only exception is when the Lake temperature is close to 0°C. In this case the IHC water may be near 4°C, the temperature of maximum density, and the plume will tend to sink. Such a sinking plume has been observed in January (Snow[10], p. 135).

After the plume has moved a few km, its subsequent vertical and lateral mixing is expected to depend on turbulent diffusivity in the Lake. We made an attempt to apply the diffusion model of Wnek and Fochtman[12] and found that with assumed constant diffusivities the calculated plume concentrations fell off more rapidly with distance than the measured concentrations. Wnek[12] had previously obtained more reasonable results using a diffusivity that varied with distance to the 4/3 power. Further effort would be needed to resolve this question.

COMPARISON OF PLUME AND NEAR-SHORE WATER POLLUTION

Based on the measured dilution factors in the plume, the study (Snow[10]) recommended reductions of pollutants such as NH3-N to meet water quality limitations in the harbor within 1-2 km of the mouth of the IHC.

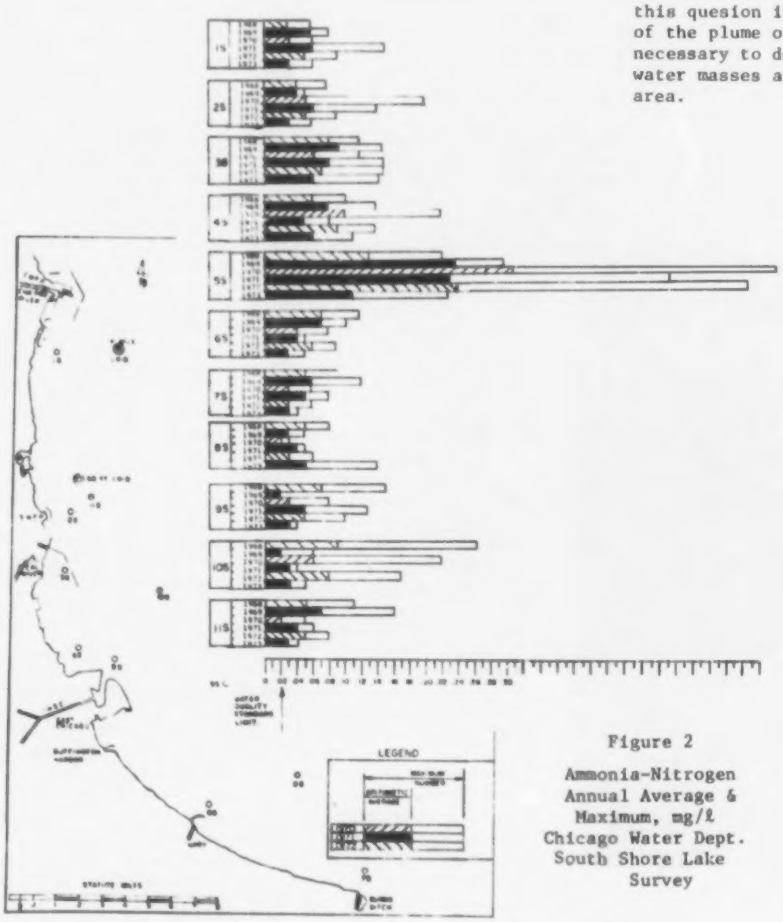

Figure 2

Ammonia-Nitrogen Annual Average & Maximum, mg/ℓ Chicago Water Dept. South Shore Lake Survey

At this stage a difficulty was encountered, because the water surrounding the plume frequently exceeds NH3-N standards for the Lake, as can be seen from Figure 2. Since the near-shore water practically never meets the open-Lake standard of 0.02 mg/ℓ, this standard cannot be met by diluting the plume with near-shore water. Less-stringent Indiana standards apply for the "inner harbor", which extends 1 km from the mouth of the IHC, but even these are difficult to meet by dilution with near-shore water.

A case could be made for not requiring the IHC effluents to be reduced to meet the Lake standards, since water outside the plume does not meet the standards. However, this argument ignores the possibility that the near-shore NH3-N concentrations may result from previous effluents, which are no longer identifiable as a plume. This is suggested by examining Figure 2, which shows that the NH3-N concentrations are higher near the IHC, and gradually decrease with distance from the IHC. Thus, although studies of the plume behavior have been successful to some extent in determining the effects on Lake water quality, we should now turn attention to effects over a wider scale of time and space.

Palmer[7] reported surveys of chloride and of phosphorus in the near-shore waters of Lake Superior near Thunder Bay, and found that the residence time of pollutants in the near-shore area was 40 days. If the residence time in the Calumet area is similar, then the NH3-N that is found in these near-shore waters may result from the effluents in the Calumet area. To answer this quesion it is not enough to determine the behavior of the plume over a period of a few hours, but it is necessary to determine the motion and dispersion of water masses as long as they remain in the near-shore area.

NEAR-SHORE CURRENTS

Knowledge of the near-shore water currents is needed to understand the eventual fate of these effluents. There have been few previous measurements of the near-shore currents, although there have extensive studies of the currents in deeper waters of Lake Michigan (FWPCA[2]). Snow[10] reported data from current meters installed near the IHC mouth by Argonne National Laboratory under subcontract. The meters used had reversible shrouded impellors designed to cancel out wave motions that would otherwise interfere with measurements in depths less than 10 m. Figure 3 presents some of the data. It was concluded that the current generally follows the shore, in the same general direction as the wind (thus differing from the more complex behavior of currents farther out in the Lake.) The speed ranges up to 20 cm/sec, and drops to zero at times when the current changes direction. These current measurements indicate that the near-shore water generally flows up and down the shore. This situation is similar to that in a tidal estuary, where pollutants are observed to move up and down the estuary.

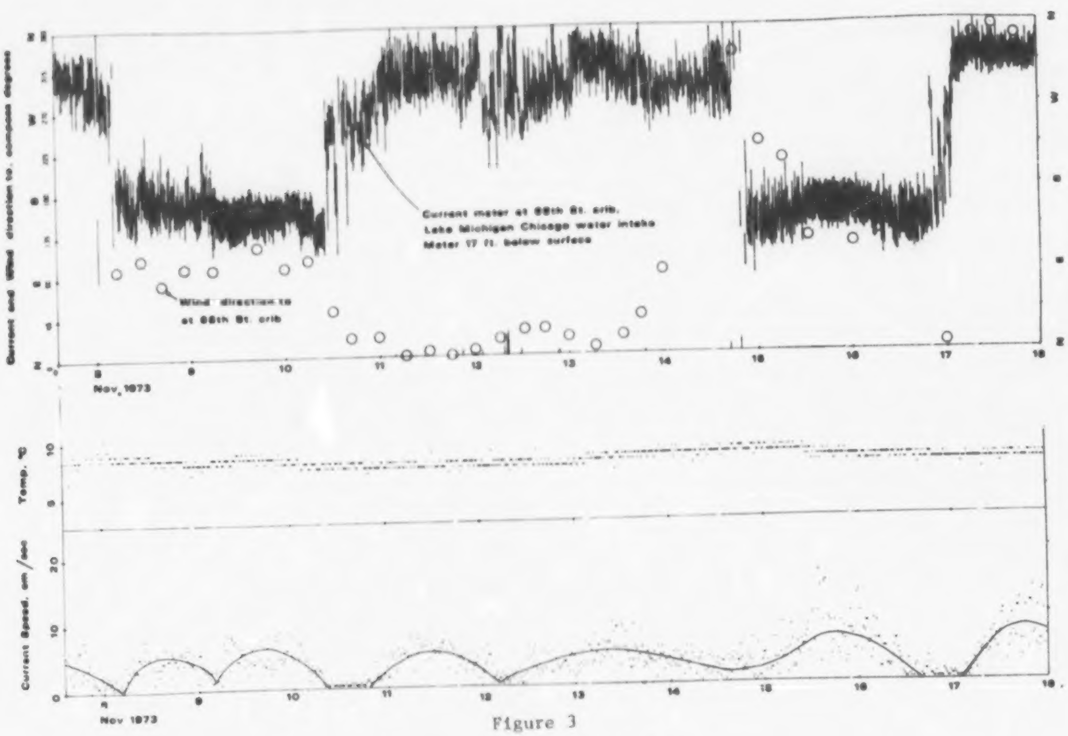

Figure 3

A Sample of Current Meter
Data From Calumet Area

Further evidence of motion of near-shore waters is obtained by observing the turbidity patterns of the water. Surface waves stir the bottom to a depth of about half the wavelength, or about 2-22 ft (Verber[11]). Figure 4 is a Landsat photo showing sediment patterns that indicate the movement of near-shore waters toward the south.

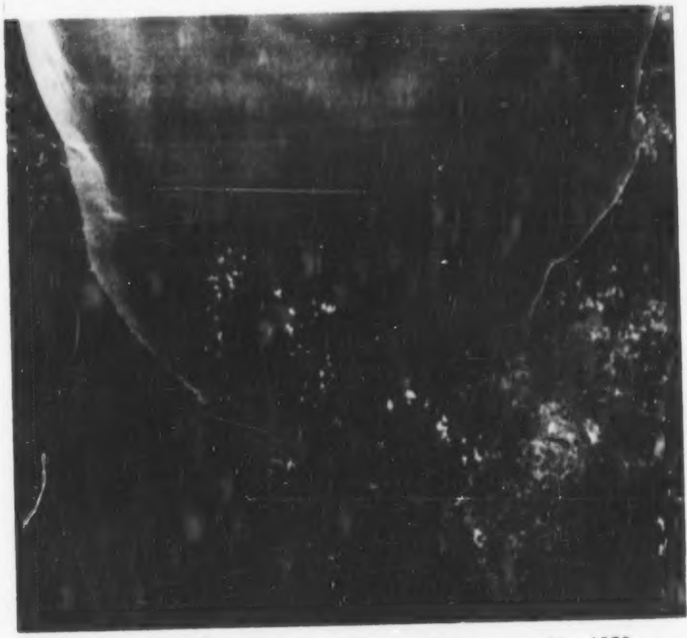

Figure 4. Landsat Photo of Lake Michigan, Aug. 21, 1973. Turbidity patterns indicate motion of near-shore waters. Lake bottom cannot be seen.

MODELLING ATTEMPTS

Current action in Lake Michigan is more complex than in the shallower Great Lakes. For this reason hydrodynamic models developed for other Great Lakes appear not to be applicable. The main current patterns in deep water of Lake Michigan have been identified and correlated with physical processes that cause the currents (FWPCA[2], and other references given by Snow[10]). Most of the current measurements were done in deep water, because the early current meters were subject to interference by waves in shallow water. It has been found (Verber[11], FWPCA[2]) that the near-shore currents may follow a different pattern from currents in deeper water. Figure 3 represents some of the few data in near-shore waters, and these data indicate that the near-shore currents follow the wind more directly than the deep-water currents.

Katz and Schwab[5] attempted to model dispersion of pollutants by applying a hydrodynamic model previously developed by Kizlauskas and Katz[6]. They predicted currents near shore that follow the wind direction; but the predicted currents in deeper water sometimes go in the wrong direction, when compared with data from FWPCA[2]. Katz and Schwab[5] combined this hydrodynamic model with a dispersion model by dividing the Lake into 10-km square cells. The near-shore water was given no special treatment. Calculations for the dispersion of effluents from the IHC during a period of alternating wind directions showed that the pollutants tended to remain in the general area, although they were not confined to the near-shore region. Whether the method of calculation would give more detailed results in the near-shore area if the grid size were finer, has not been determined.

Some general hypotheses concerning the behavior of the near-shore waters can be gleaned from observations of the current data, the turbidities, and temperatures, and the pattern of pollutants. It appears that a demarcation often occurs as seen in Figure 4 between the near-shore and deep water at a distance of 5 to 10 km from shore. This corresponds to a depth of 10 to 20 m, the location where the summer thermocline intersects the bottom (FWPCA[2], p. 125). The demarcation can be sharp or diffuse. Water in this region drifts up and down the shore with a speed of 5 to 10 cm/sec with a reversal frequency of 12 hrs to 4 days (Snow[10], pp. 120-125), during which time it can travel a distance of 2 to 35 km. Mixing can be expected at the outer boundary of the near-shore water, and this might be modelled like a boundary layer. However, since the depth is only 10 to 20 m at the outer boundary, while the width is 5 to 10 km, it will take a long time for mixing to penetrate to the shore. A more plausible mechanism for eventual dispersion of pollutants is the intermittant flow of near-shore waters to the southern tip of the Lake, where they may meet a current from the eastern shore, and hence mix out into the Lake. This is only a hypothesis, since details of such a flow pattern have not been established.

Sudden replacement of the near-shore water by cold, clear, and much purer deep-lake water is occasionally observed. Such incidents may result from upwelling, caused by unusually strong off-shore winds. The fact that this occasionally happens is evidence that during the rest of the time the near-shore residence time is long.

RECOMMENDED INVESTIGATION

It is the thesis of this paper that measurements of the behavior of the near-shore waters are needed to form the basis for dispersion modelling. The objective should be to follow the motion of the water masses, and to determine their residence time and trajectory in the area.

To obtain data needed to form the basis for dispersion modelling, the following simultaneous measurements are needed over a period of a few weeks: 1) Current meters installed 1 and 3 km from shore at 3 locations in the area, plus a few deep-water locations. 2) Analysis of satellite photos showing turbidity effects. Landsat passes occur so infrequently that few photos will be obtained during any measurement period. Earlier photos can be studied, to correlate evidence of shore current patterns with wind records. 3) Aerial surveillance can provide photos of the near-shore area twice daily from an altitude of 20,000 to 30,000 ft, and motion of plumes and sediment can be observed and measured. 4) Periodic launching into the IHC plume of markers that can be tracked from aerial photos and perhaps by radio. Markers should be designed to float just below the surface so that they follow the water mass and not directly affected by winds. 5) Measurement of a few water quality parameters, such as NH3-N, Fe, O_2, temperature, and turbidity. Samples can be taken at 5 water intakes twice daily, and from a boat at a few additional sites, preferably near the floating markers, to follow the movement and dispersion of water masses. 6) Recording of wind conditions at existing Lake stations.

Expected results of such a study will be measurement of residence time and dispersion of effluent water masses in the near-shore area, and measurement of the mixing with deeper water under measured wind conditions. These data would make it possible to develop a model for the dispersion in terms of a boundary layer or other model.

A field measurement program such as this would require cooperative efforts of several organizations, to provide current meters, aerial surveillance, water quality measurements, and data analysis and modelling. Several agencies have an interest in such measurements on Lake Michigan, and a program such as this could provide a framework for a cooperative investigation.

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A RIVER BASIN PLANNING METHODOLOGY FOR STREAMS WITH DISSOLVED OXYGEN AND EUTROPHICATION CONSTRAINTS

by

Thomas M. Walski, Sanitary Engineer
Army Corps of Engineers - Environmental Effects Laboratory - Vicksburg, MS. 39180
and
Robert G. Curran, President
Curran Associates, Inc. - Engineers and Planners - Northampton, MA 01060

Summary

Optimal Waste Load Allocation Program 2 (OWLAP2) is a user-oriented optimization model which selects wastewater treatment levels to meet water quality constraints at least cost. This program solves the problem faced by river basin planners, who by merely insuring that each wastewater discharge meets effluent standards, will still be unable to meet water quality standards. This program selects the least cost combination of additional treatment in the basin that will insure that water quality standards will be met.

OWLAP2 first simulates water quality in the reaches of the river under consideration. It then perturbs the initial conditions to determine the sensitivity of water quality to changes in effluent. It uses these sensitivities as inputs to an algorithm for linearizing non-linear systems so that they can be optimized utilizing linear programming.

Scope of Problem

A flowing stream provides many valuable services to those who live along its shores as it can be utilized as a source of drinking water, a means of transportation, a location for recreation and a route for removing waste material from a population center. With increasing population it had become obvious that if the stream was utilized excessively for waste removal, this function would interfere with other uses. This situation eventually reached the point where government intervention was necessary to reduce the waste load to acceptable levels.

Unfortunately, governmental boundaries were generally not established along those of the river basins and it was difficult to efficiently reduce the waste loads to acceptable levels. Realizing this, various governmental organizations attempted working together to effectively manage the nation's rivers, and it was found that sound planning can decrease waste reduction costs.

With passage of the 1972 Amendments to the Federal Water Pollution Control Act (PL 92-500), the United States became committed to "encouraging and facilitating the development and implementation of areawide waste treatment management plans." With this law, wastewater treatment is emphasized as the method of choice for achieving water quality goals. Once one has established wastewater treatment as the method for achieving water quality goals in a river basin system, some tools are required for analysis of the system to best employ the treatment efficiently. The systems are so complex that a plan based on experienced guesswork will not be sufficient. Instead, the tools of operations research appear to supply the most useful method for analyzing such complex systems and arriving at rational engineering designs for wastewater treatment facilities. Granted, there are a multitude of engineering judgements which must be considered in the basin plan, but the techniques of operations research should provide a comprehensive framework for making these judgements.

It is fortunate that river basin planning should come to the fore at the time when digital computer technology is currently available to solve a broad spectrum of large problems. This allows the planner to handle a wider range of problems than could be attempted without computer assistance.

The most powerful of operations research tools is linear programming. It allows one to handle a wide variety of very large problems in a reasonably small amount of computer time. Linear programming will therefore be employed in this study to find the "optimal" plan for wastewater treatment plant construction and improvement for a given river basin.

The word "optimal" in the previous paragraph is of great importance in this discussion as it is necessary to translate this concept into a linear mathematical function which can be optimized. This function is known as the "objective function." The form of this objective function is of crucial importance as it is a mathematical manifestation of the goals of those in the river basin. The objective function, which economists refer to as the "social welfare function," can be best described as:

$$\max\ (B-C)$$

where B = benefits
C = costs

In the cases when benefits from a public good cannot be estimated, benefit cost analysis must be abandoned in favor of cost effectiveness analysis. An example of this is national defense, where there is very little hope for evaluating benefits. In such a case cost effectiveness analysis, which involves minimizing costs for a given output, must be employed. This approach is attractive in a linear programming context in which the water quality goals can be included in the constraint equations without the need to formulate them in terms of cost.

Program Outline

OWLAP2 is a river basin planning program which has as its objective function minimization of wastewater treatment costs while maintaining at least a minimum level of water quality. In addition to considering BOD-DO which exhibit essentially linear behavior, OWLAP2 can optimize such parameters as nutrients which exhibit complex dynamics. OWLAP2 determines the optimal treatment level for BOD, organic nitrogen, ammonia-nitrogen, nitrate-nitrogen and phosphate-phosphorus. The program methodology, though, can be applied to other interactive systems fairly easily.

OWLAP2 uses two criteria for judging water quality levels - dissolved oxygen and algal biomass. While dissolved oxygen is the water quality parameter of most interest, eutrophication may be a problem in slow moving streams. In addition to the well-known aesthetic and taste and odor problems, a large algal population may have a serious negative effect on dissolved oxygen levels. This is due to the fact that OWLAP2 is a steady state model but large algal populations which produce oxygen during the day and consume it at night could cause serious diurnal oxygen fluctuation so that even though the steady state goals may be reached, the standards may be frequently violated. Constraining the size of the algal population can circumvent this problem.

As noted earlier, OWLAP2 handles the problem of linearizing and optimizing wastewater treatment costs for a river system in which not only dissolved oxygen but also nutrient related water quality goals must be met. The OWLAP2 package consists of a simulation program (SIMU) and the optimization routine (OWLAP2).

Since the passage of PL 92-500, effluent standards are very often so stringent that water quality constraints are not binding. There is virtually no reason to run an optimization program in this case since the degree of treatment is determined. The user can check to see if this is the case by running SIMU - the water quality model of OWLAP2 - to determine if water quality constraints will be binding. Only then need the user run OWLAP2.

This two-stage approach to determining an optimal solution serves another purpose. Since the water quality model employed in OWLAP2 is quite complex and requires knowledge of a large number of rate constants, it is desirable to test the model to see if it fits river data before attempting to run it. SIMU allows the user to do this testing at a much lower cost than OWLAP2.

The stream standards for OWLAP2 are enforced in terms of meeting a given minimum dissolved oxygen concentration and a maximum algal biomass concentration (algal biomass is expressed in terms of chlorophyll-a). The water quality parameters considered in SIMU and OWLAP2 are BOD, ammonia-N, nitrate-N, phosphate-P, organic nitrogen, dissolved oxygen and algal biomass. The water quality goals are met by reducing the amount of BOD, ammonia, nitrate or phosphate discharged in accord with the cost minimization objective.

The water quality model employed in SIMU and OWLAP2 is based on several sources including the work of O'Connor, Thomann and DiToro,[1] and Chen and Orlob.[2] The overall model is shown in Figure 1. If the user finds that the model does not accurately describe the system under consideration, he is encouraged to modify the model, during the running of SIMU, so that it does.

Since the differential equations describing the algal kinetics are non-linear, it was virtually impossible to directly convert the water quality dynamics into a linear program form. Griffith and Stewart[3] presented an algorithm for linearizing problems of this type. The linearization involves doing a Taylor expansion about the previous solution (based on the effluent standards initially). The method also checks to insure that the solution is not greatly different from the initial solution since the equations may be linear only over a small range.

The methodology of utilizing the OWLAP2 and SIMU programs is given in Figure 2. The OWLAP2 program consists of a main calling (OWLAP2) program and three subroutines:

BUILD:	constructs the water quality constraints for the linear programming problem;
COST:	sets up cost vector for optimization;
LP:	determines the optimal solution to the linear programming problem.

Optimization Routine

The optimal solution to the problem is determined using a linear programming formulation. The general form of the linear programming problem is:

$$\max Z = \underline{c}\,\underline{x} \qquad (1)$$

$$\text{subject to:} \quad A\,\underline{x} \le \underline{b} \qquad (2)$$

$$\underline{x} \ge \underline{o}$$

Equation (1) is known as the objective function (i.e. the mathematical expression to be optimized). Equations (2) are the constraint equations (i.e. the mathematical expression of the water quality effluent, or other standards to be met).

There exist numerous programming packages which solve the linear programming problem. The most commonly employed programs are those which utilize the "simplex" or "revised simplex" method. These methods are reliable but somewhat slow.

Another approach is a primal-dual algorithm which can

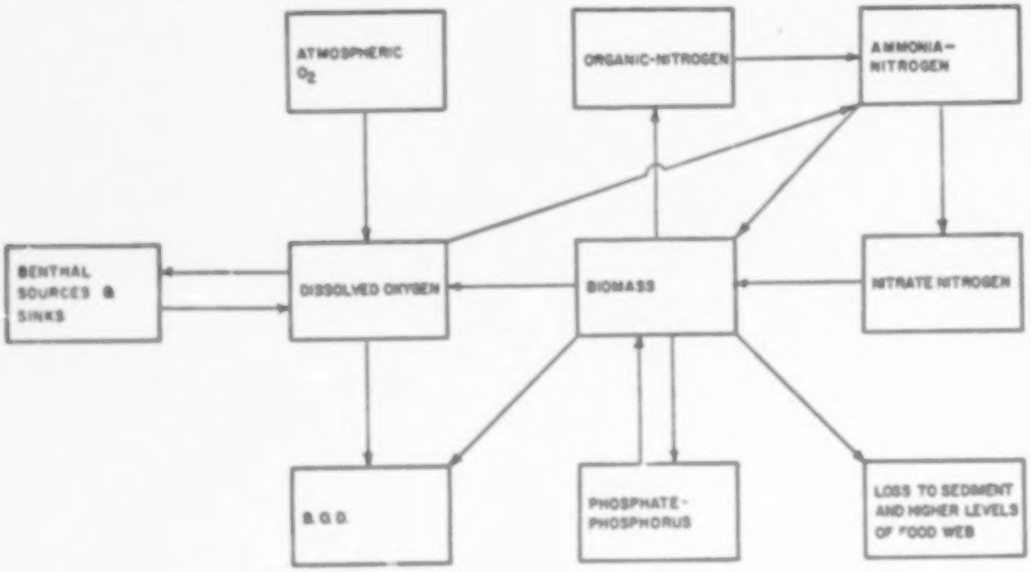

Figure 1: Water Quality Model

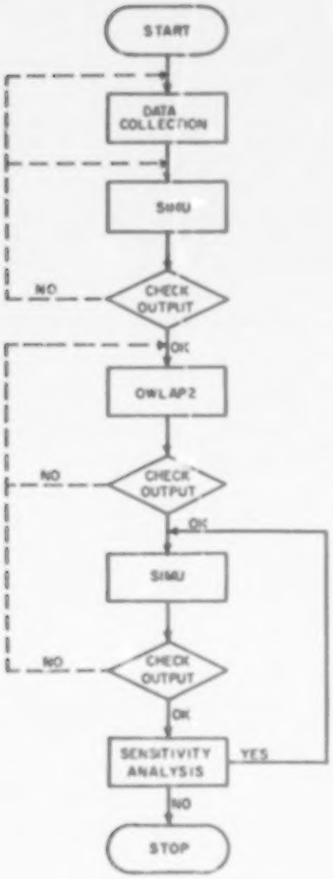

Figure 2: OWLAP2 Outline

arrive at an optimal solution in a shorter time than a simplex or revised simplex code can. For OWLAP2, the MINIT (minimum iterations) algorithm developed by Salazar and Sen[4] and translated from ALGOL to FORTRAN by this investigator were employed. It combines the features of being easy to use and not requiring a great deal of computer time or payment of rental fees.

OWLAP2 does not fit precisely into the form of the classical linear programming problem. OWLAP2, though, models the behavior of nutrients which cannot be accurately described using linear equations. Therefore, the nonlinear nutrient models must be linearized.

If the simulation portion of the program indicates the necessity to further improve treatment beyond the effluent limits, the cost minimization for the additional treatment is performed as follows:

$$\text{Maximize } G = c_1x_1+c_2x_2\ldots+c_kx_k \qquad (3)$$

subject to:

$$g_i(x_1,x_2\ldots x_k) \le b_i \qquad i = 1,2,\ldots,2m \qquad (4)$$

The x's are the decision variables (amount of pollutant discharged)

The c's are cost constants.

The b_i's are the requirements constants

2m is the number of constraints and m is the number of possible critical points as there is a dissolved oxygen and algal biomass constraint at each critical point.

k is the number of decision variables.

The superscript ° denotes values of the variables at the initial solution (i.e. only effluent constraints utilized).

The problem may be linearized by using a Taylor expansion around a vector $\underline{x}^\circ = (x_1^\circ, x_2^\circ\ldots x_k^\circ)$ for the nonlinear constraints.

This gives: $$\text{Maximize } G = \sum_{r=1}^{k} [c_rx_r^\circ - c_r(x_r^\circ - x_r)] \qquad (5)$$

subject to: $$g_i(\underline{x}^\circ)+\sum_{r=1}^{k} (x_r^\circ - x_r)\frac{\partial g_i(\underline{x}^\circ)}{\partial y_r} \le b_i \quad i=1,2,\ldots 2m \qquad (6)$$

if one makes the $\Delta x_i=(x_i^\circ - x_i)$ terms small enough,

$$\frac{\partial g_i(\underline{x}^\circ)}{\partial x_j} = w_{ij} \qquad (7)$$

The w_{ij} are constant. Equations (5) and (6) can now be rewritten as:

$$\text{Maximize } (G-v_*)=\sum_{r=1}^{k} -c_r\Delta x_r \qquad (8)$$

subject to: $$\sum_{r=1}^{k} w_{ir}\,\Delta x_r \le (b_i - v_i) \quad i=1,2,\ldots,2m \qquad (9)$$

where $$v_*=\sum_{r=1}^{k} c_rx_r^\circ$$

$$v = g_i(\underline{x}^\circ)$$

Since the g_i's are nonlinear, the w_{ij} terms are constant only for small values of Δx. To guarantee that these are indeed small, it is necessary to include constraints of the form:

$$\Delta x_j \le m_j \qquad j=1,2,\ldots,k \qquad (10)$$

where m_j is the maximum value for Δx_j. The size of m_j's was determined during the model testing and sensitivity analysis.

Equations (8), (9), and (10) completely describe the optimization problem. Griffith and Stewart suggest that if one of the Δx_j's is equal to m_j then one should use that solution as the starting point for another run with new values for $\underline{x}^\circ$, $\underline{v}$ and w_{ij}.

Since the Δx_j are always positive in this problem (one never wants to increase cost), the m_j take on added meaning. $x_j^\circ - m_j$ is the lowest value attainable for effluent concentration for any pollutant (BOD, NH_3-N, NO_3-N, PO_4-P). That means that this program is applicable only where the difference between the initial solution and the best effluent is small. This will be assured when effluent standards have been set for phosphorus and nitrogen.

The problem is now in a form in which it can be inserted into the linear programming algorithm to be used. Once the simulation routine has been run, the user must select the reach and step at which the constraint equation will be enforced. These should be the critical reaches of the river. After selecting these the computer calculates the w_{ij}'s for each critical point. Since the program calculates the waste discharge, the user does not know beforehand where the critical point of the river will be so he must run the model for several likely candidates. The problem is then organized into the format shown in Figure 3.

Water Quality Model

Algal Kinetics

The model employed to describe algal kinetics is essentially:

$$\frac{d\,(AB)}{dt} = \text{GROWTH-DEATH-LOSS} \qquad (11)$$

where AB = Algal biomass concentration.

The growth of algae can be given by:

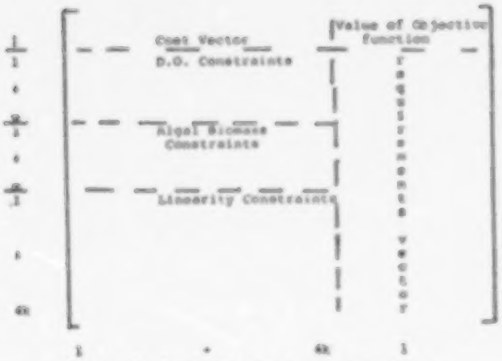

Figure 3: Form of Linear Programming Input

(k = number of discharges)
(m = number of critical points)

$$\text{GROWTH} = \text{RATE} \times \text{AB} \tag{12}$$

The RATE of algal growth can then be given by the Monod relation:

$$\text{RATE} = K_B \left(\frac{NO_3+NH_3}{S_N+NO_3+NH_3}\right) \left(\frac{PO_4}{S_P+PO_4}\right) \left(\frac{S_C}{S_C+AB}\right) \tag{13}$$

NO_3 = nitrate-nitrogen concentration
NH_3 = ammonia-nitrogen concentration
PO_4 = phosphate-phosphorus concentration
S_N = half saturation constant for nitrogen
S_P = half saturation constant for phosphorus
S_C = constant for algal self-shading

The algal death rate is a linear function of algae present. This model can easily be altered for systems in which algal die-off follows different patterns. Algal loss differs from death in that loss represents the algae and nutrients being removed from the system (usually up the food chain). Death, on the other hand, implies that the nutrients are fed back into the system.

Biochemical Oxygen Demand

BOD can be removed from the system by oxidation at rate K_1, or sedimentation at rate K_3. Aside from discharges at wastewater treatment plants and the BOD carried in by tributaries, the only BOD source is death of algae. The BOD considered is ultimate carbonaceous BOD. The following formula is employed:

(BOD contribution = (death of algae as chlorophyll-a from algae)

$$= (\text{DEATH}) \frac{78.4 \text{ gr BOD}}{\text{gr dead chlorophyll-a}} \tag{14}$$

BOD kinetics can be described by:

$$\frac{d\,\text{BOD}}{dt} = -(K_1+K_3)\text{BOD}+78.4(\text{DEATH}) \tag{15}$$

DEATH = k_DAB
K_D = rate constant for algal death

Ammonia Nitrogen

Ammonia nitrogen is formed as organic nitrogen, is broken down, and can either be oxidized to nitrate and nitrite or used as a nutrient by algae. This model does not explicitly consider the oxidation of ammonia to nitrite but rather considers the overall reaction as given below:

$$2NH_3+4O_2 \xrightarrow{\text{bacteria}} 2NO_3^-+2H^++2H_2O \tag{16}$$

The kinetics of ammonia are given below as:

$$\frac{d(NH_3)}{dt} = K_{on}(ON)-K_n(NH_3)-\frac{\text{GROWTH }(NH_3)7.2}{(NH_3+NO_3)} \tag{17}$$

ON = organic nitrogen concentration
K_{on} = rate constant for oxidation of organic nitrogen

Nitrate Nitrogen

Nitrate nitrogen is formed by oxidation of ammonia at rate K_n and is used as a nutrient for algal growth. The kinetics of nitrate are given by:

$$\frac{d(NO_3)}{dt} = K_n(NH_3) \quad \frac{\text{GROWTH }(NO_3)7.2}{(NH_3+NO_3)} \tag{18}$$

Nitrate reduction to gaseous nitrogen is not considered to be significant but can be included in the model if low dissolved oxygen levels are to be expected in a reach.

Phosphate Phosphorus

Phosphate-phosphorus has as its source wastewater discharges and release of phosphorus from dying algae. The kinetics of phosphate are given below:

$$\frac{dP}{dt} = 1.66\ (\text{DEATH} - \text{GROWTH}) \tag{19}$$

The constant 1.66 is derived from the conversion by Megard.[5]

$$\frac{1.66 \text{ gr P}}{\text{gr chlorophyll-a}} \tag{20}$$

If removal of phosphorus by sediments is significant, it can be easily included in the model.

Organic Nitrogen

Organic nitrogen as referred to in this problem is organic nitrogen, not as living biomass (e.g. amino acids and polypeptides released from decaying biomass). Organic nitrogen decays to ammonia and is formed by decaying living matter. The kinetics of organic nitrogen are given below:

$$\frac{d(ON)}{dt} = -K_{on}(ON) + (\text{DEATH})7.2 \tag{21}$$

The constant 7.2 is a conversion factor, since there are 7.2 mg organic nitrogen per every mg of chlorophyll-a, and DEATH is expressed as mg algae (as chlorophyll-a) that die per day. It is also assumed that nitrogen fixation is not significant.

Dissolved Oxygen

Dissolved oxygen is consumed in oxidation of carbonaceous BOD, organic nitrogen, and ammonia-nitrogen. It is replaced through atmospheric reaeration and algal respiration. The rates are respectively K_1, K_n, K_2, and K_r. The kinetics of dissolved oxygen are given by:

$$\frac{d(DO)}{dt} = -K_1(\text{BOD})-4.57K_n(NH_3)+K_2(C_s-DO)+K_r(\text{GROWTH})-SR \tag{22}$$

C_s = mg/l chlorophyll-a
K_1 = rate constant for oxidation of BOD
K_2 = rate constant for atmospheric reaeration
K_n = rate constant for nitrification
K_r = rate constant for algal respiration
SR = other oxygen sources and sinks

The K's have units of 1/day except for K_r, which is in mg O_2/mg chlorophyll-a/day. The 4.57 in Equation (22) represents the gram of ammonia nitrogen to nitrate stoichiometrically.

Special Note

While OWLAP2 provides the framework for optimally allocating waste loads, the user must realize that the results of the model will only be as accurate as the model, model calibration and cost inputs allow. The program is constructed so that the model can be easily adjusted to fit virtually any one-dimensional, steady-state system. Since the model is so flexible, great care must be exercised in adjusting the model so that it will be specific for each system. This requires considerable data collection. Similarly, while typical cost data is included in the model, the user must be aware that costs will be site specific and must include accurate costs as the model is quite sensitive to these inputs.

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MODELING POLLUTANT MIGRATION IN SUBSURFACE ENVIRONMENTS

Amir A. Metry, Ph.D., P.E.
Project Manager
Roy F. Weston, Inc.
West Chester, Pennsylvania

SECTION 1
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SECTION 2
INTRODUCTION

Need for Proper Assessment of Potential Groundwater Pollution

Groundwater is one of the earth's most widely distributed and most important resources. Its quantity is estimated to be six times that of the fresh water flowing in all the streams on earth. Groundwater accounts for 20 percent of the total amount of water withdrawn from all other sources. Groundwater resources have many advantages over surface water resources because they are more widely and easily available than surface water supplies. The physical and chemical quality of groundwater is fairly uniform throughout the year. It is rarely, if ever, necessary to consider removal of sediment from groundwater.

The existing demand for groundwater as a source of conventional water supply will continue to grow; furthermore, aquifers will be considered as storage media for flood water in place of dams and reservoirs as the cost of these facilities grows progressively more expensive. With the effort to clean up streams under water pollution control acts, aquifers will be in demand as alternative means for direct and indirect disposal of both liquid and solid wastes from industrial and domestic activities.

Although not as dramatic and apparent as surface water pollution, degradation of the quality of subsurface waters is widespread. Several sources of groundwater pollution have been identified, including leachate from sanitary landfills; industrial waste seepage from storage basins; industrial waste introduced through groundwater recharge; domestic waste from septic tanks; fertilizer, pesticides, and irrigation salts leached from soils in agricultural areas, and leachate from raw materials and waste stockpiles, etc.

The successful location and operation of a waste disposal site require quantitative knowledge of how leaching fluids will migrate through an aquifer. This will depend on hydrogeologic parameters of the leachate/aquifer system, type of waste, and climatic conditions at the site area. Experimental methods are required to quantify the different parameters involved in the mass exchange between leachate and the aquifer. Among the different types of models suitable for dispersion patterns, mathematical models can be conveniently devised.

This mathematical model describes the hydrogeologic relations within a leachate/aquifer system. It is usually in the form of a second-order partial differential equation together with a set of auxiliary conditions describing the system's variables and constants. If such equations are sufficiently simplified, exact solutions may be possible. On the other hand, however, these simplifications are often physically unrealistic. Numerical solutions obtained with the aid of high-speed digital computers offer a great help for solving such equations under physically realistic assumptions.

Problem Definition

Rainfall over a waste disposal processing or storage area causes infiltration, and therefore leachate generation. Most of the states in the U. S. have net infiltration; the potential for leachate generation therefore exists in these humid areas.

Leachate containing several polluting substances leaves the waste material and travels through unsaturated media. During their travel, many of these pollutants are subject to assimilation by soils, because of the adsorption and ion exchange capacity of such materials. Attenuated leachate then leaves the subsaturated zones and enters the aquifer, where it is subject to dispersion in groundwater and to chemical reaction with earth materials.

In order to determine the impact of a waste handling or disposal facility on subsurface waters the following steps must be taken:

1. Determine quantities and characteristics of the leachate. This can be accomplished by laboratory and/or field investigations.
2. Determine the degree of leachate assimilation as it travels through unsaturated media.
3. Determine the pattern of leachate dispersion and its eventual concentrations and chemical reactions in the aquifer.

Scope and Objectives

Modeling leachate dispersion and assimilation in subsaturated and saturated media is an essential step in determining impact of waste disposal facilities on subsurface water quality.

The main objective of this study is to develop mathematical and computer models to predict leachate-pollutant migration and fate in subsurface environments. Because of the hydraulic discontinuity between subsaturated earth layers (soils) and saturated layers (aquifers), two models were developed: 1) a one-dimensional model to predict pollutant attenuation in subsaturated media (soils), and 2) a two-dimensional model to predict pollutant migration and fate in saturated media (aquifers). Four basic criteria were considered in developing these models. The models should be--

- Representative of the physical conditions of both the saturated and unsaturated media.
- Based on sound mathematical principles.
- Easy to understand and usable by engineers and scientists.
- Practical, and economical to run, on commonly used computers.

Summary of Literature Review

The literature is rich in theoretical background for dispersion of soluble matter in porous media. More work has been done in the area of dispersion in saturated media than in unsaturated ones. There is apparent agreement in the literature on the validity of partial differential equations to model pollutant dispersion and fate in porous media (soils and aquifers); however, there is still a tremendous gap between the degree of sophistication of research in this field and the actual technology used in day-to-day applications. In spite of the great research effort, almost all solid and liquid waste disposal sites are located on land without any modeling activity to determine their impact on subsurface water quality and to determine the need for, and degree of environmental controls. One reason for this great gap is the difficulty that engineers and scientists working in the field have in understanding and applying much of the existing research; unfortunately, most of the published research work ended up as research for sake of research, rather than application. Therefore, the need for easy-to-understand and easy-to-apply models utilizing easy-to-quantify field conditions (hydrogeologic parameters) is badly needed to predict pollutant fate and dispersion in soils and aquifers.

SECTION 3
MODELING POLLUTANT MIGRATION IN SUBSATURATED MEDIA

Large quantities of solid waste and hazardous waste are being disposed of by placing the material on the soil surface or by burying it in large landfills. These practices are often conducted without proper consideration of how the waste material will behave in a given soil or under specific climatic conditions. Procedures are needed to assist in site selection and to define proper management schemes for applying waste onto or below the soil surface. The procedure needs to be descriptive of how various constituents in a waste behave in a soil-water system, but simple enough to be of practical use.

Mathematical Model

This section presents an approach to these problems which may be of value. The procedure, because of insufficient research data, has not been validated and should not be applied without first comparing it to field data and experience. The physical system assumes a constant application of a leachate constituent (e.g., Cd, Pb, Hg, As, and Se) of concentration c_o (μg/cm^3 or mg/L) to the soil surface or large sources of waste in a landfill that releases a given constituent to the soil-water system at a concentration c_o. The following conceptual model was used for this investigation:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - w\frac{\partial c}{\partial z} - \frac{\rho}{\theta}\frac{\partial s}{\partial t} - Kc \qquad (3.1)$$

where:

c = constituent concentration (μg/cm^3 or mg/L) in soil solution
s = adsorbed constituent concentration (μg/g or mg/kg)
t = time (yr)
D = Hydrodynamic dispersion coefficient (m^2/yr)
z = distance (m)
w = average pore-water velocity (m/yr)
ρ = bulk density of dry soil (g/cm^3)
θ = soil water-content fraction (cm^3/cm^3)
k = transformation rate constant (yr^{-1})

The third term on the right hand side of equation (3.1) represents adsorption. An equilibrium adsorption state will be assumed with a linear relationship between solution and adsorbed solute phases. This is expressed as:

$$S = K_d c \qquad (3.2)$$

where K_d is the distribution coefficient (cm^3/g). Differentiating (3.2) with respect to time gives:

$$\frac{\partial S}{\partial t} = K_d\frac{\partial c}{\partial t} \qquad (3.3)$$

Substituting (2.2)into (3.1) and rearranging gives:

$$\left(1 + \frac{\rho K_d}{\theta}\right)\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - w\frac{\partial c}{\partial z} - Kc \qquad (3.4)$$

or

$$\frac{\partial c}{\partial t} = \frac{D}{R}\frac{\partial^2 c}{\partial z^2} - \frac{w}{R}\frac{\partial c}{\partial z} - \frac{Kc}{R} \qquad (3.5)$$

where $R = (1 + \frac{\rho K_d}{\theta})$, which is frequently referred to as retardation factor. When no adsorption occurs ($K_d = 0$), the retardation factor is unity. Note that as the retardation factor is increased above unity, the effective values for hydrodynamic dispersion, average pore-water velocity, and transformation rate are reduced. The net effect is to reduce the mobility and chemical transformation parameters of the constituents being described.

Equation (3.5) was solved for the following initial and boundary conditions:

$c = 0 \qquad x > 0 \qquad t = 0$
$c = c_o \qquad x = 0 \qquad t > 0$

The physical meaning of the boundary conditions corresponds to a situation where a soluble constituent in leachate (e.g., Cd, Pb, Hg, As, or Se) is continually supplied to a soil surface which did not contain the material initially. The chemical transformation process represents irreversible adsorption, precipitation, and/or changes in the chemical state of the constituent being described.

Mathematical Solution

The solution to (3.5), subject to the initial and boundary conditions, is

$$\frac{c}{c_0} = \frac{1}{2}\left[\exp\left\{\frac{z}{2D'}\left(w' - \sqrt{w'^2 + 4D'K'}\right)\right\}\left\{\operatorname{erfc}\left(\frac{z - t\sqrt{w'^2 + 4D'K'}}{\sqrt{4D't}}\right)\right\} + \exp\left\{\frac{z}{2D'}\left(w' + \sqrt{w'^2 + 4D'K'}\right)\right\}\left\{\operatorname{erfc}\left(\frac{z + t\sqrt{w'^2 + 4D'K'}}{\sqrt{4D't}}\right)\right\}\right] \quad (3.6)$$

where:

$w' = w/R$
$D' = D/R$
$K' = K/R$

erfc (z) is the complementary error function.

Model Parameters

The average pore-water velocities (w) used in this section to illustrate the general utility of equation (3.6) are 1.75, 0.876, 0.438, and 0.088 m/yr. The corresponding fluxes or Darcy velocities depend upon soil-water content (θ), since average pore-water velocity (w) is equal to flux or Darcy velocity divided by soil-water content by volume (θ). Therefore, the annual groundwater recharge represented by these average pore-water velocities will also depend upon the average soil-water content in the water transmission zone. The dispersion coefficient is a function of average pore-water velocity and was obtained using the following relationship from Bigger and Nielsen (to appear).

$$D = 0.022 + 0.17\,w^{1.14} \quad (3.7)$$

The transformation rate coefficients selected are 0.00876, 0.0876, and 0.876 yr^{-1}. These are, in general, small values, and may or may not be realistic parameters for leachate containing heavy metals (Cd, Pb, Hg, As, or Se).

A literature search was conducted using the reference in Copenhauer and Wilkinson (1974), but transformation rate constants (k) and distribution coefficients (K_d) are not measured or reported generally. The values used in this report are thought to represent the range that might be encountered in a natural soil environment. A K_d if not available for a given soil and leachate constituent could be measured by shaking leachate containing a known concentration of the solute with soil (e.g. at 1:1 ratio) until equalibrium, and then measuring the constituent concentration in the supernatant solution. This procedure gives the quantity of the constituent adsorbed. The ratio of equilibrium adsorbed concentration (S) to solution concentration (c) is equal to K_d. This procedure assumes that the adsorption isotherm is linear over the concentration range in question.

SECTION 4
MATHEMATICAL MODELING OF POLLUTANT MIGRATION IN AQUIFERS

In this section different mathematical models will be formulated to represent migration of pollutants generated from a waste-disposal site into saturated porous earth materials. Three major mass-transport mechanisms are included separately or simultaneously in each model:

- Molecular diffusion -- the transport of pollutants in their ionic state because of the difference in concentration levels of a given species in the aquifer.
- Convective dispersion -- the mixing of pollutants in the aquifer caused by the variation in the microscopic-pore velocities within each channel of flow, or from one channel to another.
- Chemical reaction -- the transfer of the polluting substances from their liquid carrier to the solid matrix of the aquifer. In this study the transfer of pollutants is considered in the adsorptive rather than the desorptive sense.

Simultaneous Diffusion, Convective Dispersion and Chemical Reaction Model

The rate of change of concentration $\partial c/\partial t$ can be mathematically defined for the diffusion convective dispersion models and a chemical reaction term which can be defined as the function f(c).

$$\frac{\partial c}{\partial t} = \operatorname{div}\,(D_m \operatorname{grad} c) + \operatorname{div}\,(D' \operatorname{grad} c) - v \operatorname{div} c - f(c) \quad (4.1)$$

Including the coefficients D_m and D' in one term D, the effective diffusivity, Equation (4.1), can be rewritten as

$$\frac{\partial c}{\partial t} = \operatorname{div}\,(D \operatorname{grad} c) - v \operatorname{div} c - f(c) \quad (4.2)$$

f(c) is a function of concentration,

where:

c: pollutant concentration (ML^3)
D: is the effective diffusivity (L^2T^{-1})
v: groundwater velocity vector (LT^{-1})

$f(c) = b\,(c-ms)^n$
s = concentration of polluting substance per unit weight of the solid matrix
b and M = constants
n = exponent ≤ 1

SECTION 5
NUMERICAL SOLUTION OF TWO-DIMENSIONAL MODEL OF POLLUTANT MIGRATION IN AN AQUIFER

In order to use operational methods for solving mathematical models, many oversimplifications have to be imposed in order to solve the second-degree partial differential equations describing the system: collapsing the model into a one-dimensional state, assuming homogeneity of the medium, and considering only one mechanism or two of the three mechanisms involved in the mass transport in every solution. These simplifications and assumptions, which are necessary but physically unrealistic, reduce the value and applicability of the operations solutions to real physical problems. In this section, a numerical technique is developed to solve the mathematical equation describing simultaneous diffusion, convective dispersion, and chemical reaction of pollutants into an unconfined aquifer in two dimensions under transient and steady-state conditions.

Formulation of the Finite Difference Scheme

As shown in Section 4, the dispersion equation in the x-z domain can be rewritten as:

$$\frac{\partial c}{\partial t} = Dx \frac{\partial^2 c}{\partial x^2} + Dz \frac{\partial^2 c}{\partial z^2} - u \frac{\partial c}{\partial x} - w \frac{\partial c}{\partial z} - K(c) \qquad (5.1)$$

In Equation (5.1) the different variables and parameters are defined as follows:

x and z: Cartesian coordinates in the direction of groundwater flow and vertical direction respectively (units: L)

Dx and Dz: are the effective diffusivities in the x and z directions respectively ($L^2 T^{-1}$)

u, w: are the components of pore velocities in the x and z directions respectively (LT^{-1})

K : is the coefficient of chemical reaction of the polluting substance with the porous medium (T^{-1}).

Using the backward difference equation for time,

$$\left(\frac{\partial c}{\partial t}\right)_{m,n,s} = \frac{c_{m,n,s+1} - c_{m,n,s}}{\tau} + (\tau) \qquad (5.2)$$

Using the central difference equation for x and z

$$\left(\frac{\partial c}{\partial x}\right)_{m,n,s} = \frac{c_{m+1,n,s} - c_{m-1,n,s}}{2h} + 0\,(h^2) \qquad (5.3)$$

$$\left(\frac{\partial c}{\partial z}\right)_{m,n,s} = \frac{c_{m,n+1,s} - c_{m,n-1,s}}{2k} + 0\,(k^2) \qquad (5.4)$$

$$\left(\frac{\partial^2 c}{\partial z^2}\right)_{m,n,s} = \frac{1}{k^2} \left[c_{m,n-1,s} - 2c_{m,n,s} + c_{m,n+1,s}\right] + 0(k) \qquad (5.5)$$

and

$$\left(\frac{\partial^2 c}{\partial x^2}\right)_{m,n,s} = \frac{1}{h^2} \left[c_{m-1,n,s} - 2c_{m,n,s} + c_{m+1,n,s}\right] + 0(h) \qquad (5.6)$$

where:

h, k, τ : numerical increments of x, z and t, respectively.

m, n, s: nonnegative integers corresponding to x, z and t coordinates respectively.

Substituting Equations (5.2) - (5.6) into Equation (5.1):

$$\frac{1}{\tau}(c_{m,n,s+1} - c_{m,n,s}) = \frac{Dx}{h^2}(c_{m-1,n,s} - 2c_{m,n,s} + c_{m+1,n,s}) + \frac{Dz}{k^2}(c_{m,n-1,s} - 2c_{m,n,s} + c_{m,n+1,s}) - \frac{u}{2h}(c_{m+1,n,s} - c_{m-1,n,s}) - \frac{w}{2k}(c_{m,n+1,s} - c_{m,n-1,s}) - k\,c_{m,n,s} \qquad (5.7)$$

Rearranging Equation 5.7, the explicit form of the difference equation can be written as follows:

$$c_{m,n,s+1} = c_{m,n,s} + \frac{\tau Dx}{h^2} c_{m-1,n,s} - \frac{2\tau Dx}{h^2} c_{m,n,s} + \frac{\tau Dx}{h^2} c_{m+1,n,s} + \frac{\tau Dz}{k^2} c_{m,n-1,s} - \frac{2\tau Dz}{k^2} c_{m,n,s} + \frac{\tau Dz}{k^2} c_{m,n+1,s} - \frac{\tau u}{2h} c_{m+1,n,s} + \frac{\tau u}{2h} c_{m-1,n,s} - \frac{\tau w}{2k} c_{m,n+1,s} + \frac{\tau w}{2k} c_{m,n-1,s} - \tau K c_{m,n,s} \qquad (5.8)$$

Introducing the non-dimensional parameters α_x, α_z and β_x, β_z, and κ as:

$$\alpha_x = \frac{\tau Dx}{h^2}, \text{ and } \alpha_z = \frac{\tau Dz}{k^2} \qquad (5.9)$$

$$\beta_x = \frac{\tau u}{h} \quad \beta_z = \frac{\tau w}{k} \qquad (5.10)$$

$$\kappa = \tau K \qquad (5.11)$$

Substituting Equations 5-9, 5-10 and 5-11 into Equation 5-8 and rearranging,

$$c_{m,n,s+1} = c_{m,n,s}\,|1 - 2\alpha_x - 2\alpha_z - \kappa| + c_{m-1,n,s}\,|\alpha_x + 0.5\beta_x| + c_{m+1,n,s}\,|\alpha_x - 0.5\beta_x| + c_{m,n-1,s}\,|\alpha_z + 0.5\beta_z| + c_{m,n+1,s}\,|\alpha_z - 0.5\beta_z| \qquad (5.12)$$

The Computational Molecule for the x-z domain can be written as:

$$c_{m,n,s+1} = c_{m,n,s}\,|1 - 2\alpha_x - 2\alpha_z - \kappa| + \text{Left}\,|\alpha_x + 0.5\beta_x| + \text{Right}\,|\alpha_x - 0.5\beta_x| + \text{Up}\,|\alpha_z + 0.5\beta_z| + \text{Down}\,|\alpha_z - 0.5\beta_z| \qquad (5.13)$$

Left, Right, Up, and Down represent the concentrations of the pollutants with respect to the specific grid point $c_{m,n,s}$ in the finite difference scheme.

Conditions for Stability of the Numerical Solution

The necessary conditions for stability of the numerical scheme can be written as

$$\left(\frac{\tau Dx}{h^2} + \frac{\tau u}{h}\right) + \left(\frac{\tau Dz}{k^2} + \frac{\tau w}{k}\right) < 1 \qquad (5.14)$$

and

$$\tau K < 1 \qquad (5.15)$$

SECTION 6
DEFINITION OF PARAMETERS

Unsaturated Model

The parameters that appear in the mathematical model for subsaturated media are those found in the following equation:

$$\frac{\partial c}{\partial t} = \frac{D}{R} \frac{\partial^2 c}{\partial z^2} - \frac{w}{R} \frac{\partial c}{\partial z} - \frac{K}{R} c \qquad (6.1)$$

c, t, z, D and K are similar to the parameters for the saturated flow media and are discussed in the following section.

R is known as the retardation factor and is equal to $(1 + \frac{\rho K_d}{\theta})$

ρ is the bulk density of dry soil or earth materials (g/m^3) and can be estimated for each type earth materials or quantified through laboratory testing of undisturbed core samples, or by correlation with the degree of soil saturation

K_d is the distribution coefficient (cm^3/g). The value of K_d is a leachate/soil specific and could be measured in the laboratory by shaking leachate containing a known concentration of the solute with soil (e.g. 1:1 or 1:10 ratio) until equilibrium is reached and then measuring the constituent concentration in the supernatant. The ratio of equilibrium adsorbed concentration (s) to solute concentration (c) is equal to K_d, for linear adsorption isotherms.

θ water content, by volume (ml of water per cm^3 of soil)

S concentration of adsorbed phase (mg/g soil)

Saturated Model

The parameters that appear in the mathematical model for saturated media are those found in the following equation:

$$\frac{\partial c}{\partial t} = Dx \frac{\partial^2 c}{\partial x^2} + Dz \frac{\partial^2 z}{\partial z^2} - u \frac{\partial c}{\partial x} - w \frac{\partial c}{\partial z} - Kc \quad (6.2)$$

The concentration, c_o, of each polluting substance in the leachate as it enters the aquifer is determined by applying the mathematical equations 3.1 and 3.6 presented in Section 3. The saturated media model predicts concentrations (c) at various locations in the aquifer (identified by x,z coordinates) for differenct values of time, t.

Time (t): Time is the duration of travel of polluting substances in the aquifer. Time can be described as: a) a buildup period, in which the concentration of a certain contaminant increases; b) a steady state period, in which the concentration remains constant; or c) recovery period, in which the concentration starts to decline with the passage of time. The representative time for a computer run will vary, depending on aquifer hydrogeologic character, from several months to ten years. Time increments vary from several days to several months.

Space Coordinates (x and z): These are taken in the direction of groundwater flow and perpendicular to it, respectively. In the computer runs, the spatial domain in the direction of flow extends from a few hundred feet to a few miles, and in the vertical direction it extends from a few feet to a few hundred feet, depending on the characteristics of the aquifer. The increment varies from 10-1000 feet in the direction of flow, and 1-10 feet perpendicular to it.

Effective Diffusion Coefficients (D_x and D_z) are a function of molecular diffusion coefficients and pore velocities (u and w). Their numerical values vary from from a fraction to several sq ft/day, depending on type of aquifer materials and pore velocities.

Chemical Reaction Coefficient (κ): This value is expressed as a linear function of the concentration. In this study, κ is considered in the sense of pollutant removal from solution into the solid matrix. It is difficult, however, to develop a single value for this function since it is dependent on geophysical and geochemical properties of the aquifer and on groundwater/leachate chemical interaction. The value of κ is usually on the order of a small fraction of Day^{-1} for most aquifers, and it increases with increases in reactive materials (e.g., clay or salts) content in the aquifer materials. Chemical reaction coefficients can be determined using laboratory columns (lysimeters).

SECTION 7
COMPUTER SIMULATION

General Considerations

Pollutant migration through subsaturated soil and saturated aquifers has been dealt separately using Equations (3.1) and (5.1), respectively. Equation (3.1) has been solved analytically and the solution is given by Equation (3.6). For saturated media, Equation (5.1) has been solved numerically using finite difference technique. The finite difference form of Equation (5.1) is given by Equation (5.6). The conditions of convergence of solution of finite difference Equation (5.6) to differential equation (5.1) are given by Equations (5-14) and (5-15). A program has been developed to solve Equation (5.6) numerically using a high speed digital computer using proper initial and boundary conditions.

The differential equation for substaturated soil layers (Eq. 1.1) will be solved first to find the concentration of a pollutant as it enters the interface of the subsaturated and saturated layers. This would constitute one of the boundary conditions (at z = 0) for the solution of the saturated model. The concentration of the pollutant at other boundary conditions is assumed to be equal to background condition. The initial condition of pollutant concentration at all the x - z grid points at time t = 0 has been assumed to be equal to the background concentration.

The computer simulation is expressed as two-dimensional concentration profiles which can be oriented in either the vertical or the horizontal domain, under transient or steady-state conditions.

Program Logic

When the initial and boundary condition values of pollutant concentration in two saturated aquifers are known, the concentration of pollutants at all the x - z grid points at t = 0 are known. The computation of concentration for all x-z grid points for the next time internal, Δt, would be done using the finite difference equation (5.6). In a similar manner, a step-by-step solution for the pollutant concentration at all x-z grid points for various time intervals may be obtained.

The procedure of "marching solutions" is repeated for progressing time intervals up to the required time period for which the results are desired. The selection of finite difference grid intervals should be made in such a way that the stability conditions (Equations 5.14 and 5.15) are satisfied. The program has been written in FORTRAN IV and is installed in the Weston computer system.

Input Requirements

The input data required for computation consist of grid characteristics, initial and boundary concentrations of pollutants, program operation and control data, and aquifier characteristics such as velocities and diffusion coefficients in the x and z directions and the coefficient of adsorption. The output of the program consists of the ratio of concentration of pollutant in the two-dimensional domain for various time periods.

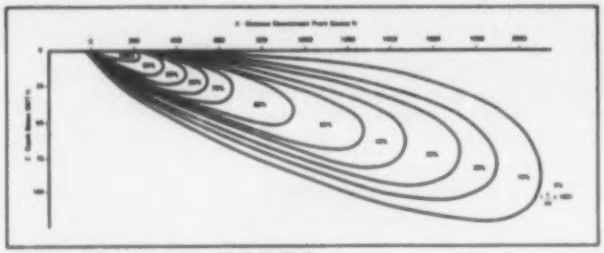

FIGURE 1 POLLUTANT ISOPLETHS (RUN 1)

Typical Run

Figures 1 through 3 are graphical presentations of computer simulation of a typical run based on the following parameters:

Number of Finite Space Increments in X Direction	=	20
Number of Finite Space Increments in Y Direction	=	20
Number of Finite Time Increments	=	52
Background Concentration of Pollutant	=	0.0100
Grid Space Size in X Direction in Feet	=	200.00
Grid Space Size in Z Direction in Feet	=	5.00
Grid Size in Time Direction in Days	=	7.00
Coeff. of Chemical Reaction of Adsorp. of Poll.	=	0.001
Effective Diffusion Coeff. in X-Direction, ft^2/day	=	4.000
Effective Diffusion Coeff. in Z-Direction, ft^2/day	=	0.50
Ground Water Flow Velocity in ft/day	=	5.00
Vertical Velocity of the Leachate in ft/day	=	0.20

Figure 1 is a plot of pollutant isopleths in the aquifer. The leachate plume dips in the aquifer, which is attributed to the vertical-component velocity vector (recharge velocity).

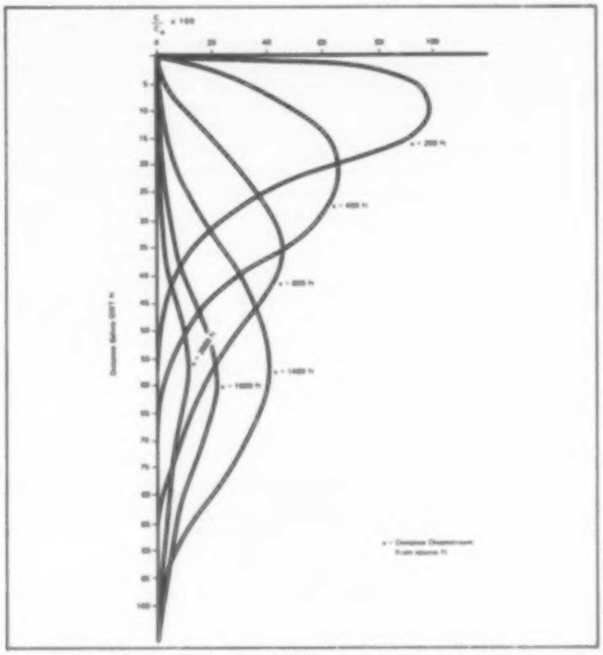

FIGURE 2 CONCENTRATION PROFILES FOR VARIOUS DEPTHS BELOW GWT (RUN 1)

Figure 2 and 3 are plots of concentration profiles for various depts below ground water and for various distances downstream of source respectively.

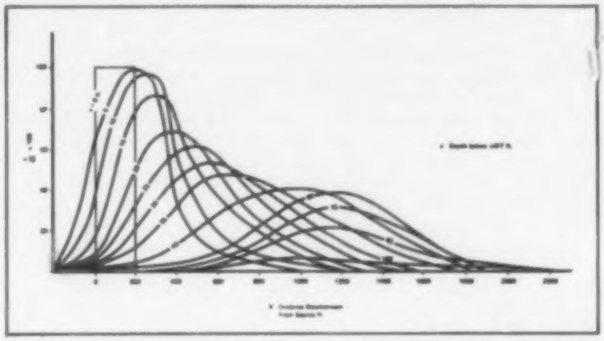

FIGURE 3 CONCENTRATION PROFILES FOR VARIOUS DISTANCES DOWNSTREAM FROM SOURCE (RUN 1)

SECTION 8
CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE RESEARCH

Conclusions

- The models developed in this study: a) have a sound mathematical basis; b) account for major mass transport mechanisms; c) are flexible and practical; and d) are accurate.
- The models can be used to simulate subsurface contamination from area sources, such as solid waste disposal sites, wastewater holding basins, wastewater or sludge application sites, raw material stockpiles and recharge of contaminated waters.
- The models can be used as a tool for water quality studies, disposal site selection and design, evaluation of environmental impact, recovery of groundwater contaminants, and planning related to subsurface water resources.
- The accuracy of predicted contamination by the models depends on the accuracy of hydrogeologic parameters used in the simulation. It is realized that quantifying such parameters is one of the most difficult tasks in simulating subsurface water contamination.

Recommendations for Future Research

- The "first generation models" developed in this study should be further tested, using field data.
- More effort is needed in defining and quantifying various hydrogeologic parameters used in the models.
- The "second generation" models should be upgraded to account for: a) multiple sources; b) heterogeneity of soils and aquifers; c) non-linearity of chemical reactions; and d) pumping and recharge in an aquiefer.
- It would be of great value to engineers and scientists in the field if the computerized solution of the models were expressed in a series of nomographs that related pollutant concentration to hydrogeological parameters of a disposal site area.

A MODEL OF TIDAL FLUSHING FOR SMALL COASTAL BASINS

Albert Y. Kuo
Virginia Institute of Marine Science
Gloucester Point, Virginia 23062

Abstract

An empirical theory is proposed to model the flushing of a small coastal basin by tidal exchange. The theory is adapted from Ketchum's[2] tidal prism concept with modification. The application of the method requires that a water body be divided into segments such that complete mixing at high tide within each segment may be assumed. Starting from the mouth, each segment is defined such that its volume at low tide equals the total tidal prism landward from the inner boundary of the segment. Therefore, each segment has a length equal to the local tidal excursion.

The flushing capability of a segment is defined as the fraction of dissolved substance removed per tidal cycle, i.e. the flushing rate, which was derived from the principle of mass-balance. The concentration distribution of an introduced pollutant was expressed in terms of discharge rate, volume, flushing rate, and decay rate. A model has been set up for the Cockrell Creek of Virginia to study a proposed 0.2 MGD STP. The model was used to project the distribution of fecal coliform bacteria and biochemical oxygen demand.

Introduction

Estuaries and coastal waters are being used more and more frequently as dumping grounds for pollutants resulting from human activities. If properly balanced with the assimilative capacity, this may be a practical use of these water bodies. However, careful planning must be executed such that the introduced pollutants will not upset the ecological balance and preclude other usage of the water bodies.

The application of water quality models has proven to be a powerful technique in water resource management. The primary results of the model are the prediction of the distribution and concentration resulting from discharge of a new pollutant, or an increase or decrease of an existing pollutant discharged to a water body. The fundamental goal of a water quality model is to represent the complex interaction of the prototype in a simplified form which not only simulates the existing conditions with accuracy but also can predict the likely consequence of a proposed change of pollutant discharge.

The majority of recent developments in the field of water quality modeling pertain to numerical mathematical modeling[1]. These models used advanced computer techniques to find solutions to the governing equations of motion and mass balance. An important feature of these models is the requirement of substantial data from prototype, either for input data or for calibration and verification of the model. The application of these models to a particular water body often involves a large investment of time and effort. In the case of small coastal basins (e.g. a coastal creek of the order of 10 km long, 100 meters width), it is usually impractical to use this kind of model to study a proposed small waste discharge. A simple tidal flushing model for small coastal basins which requires only the data of tidal range and basin topography is described in this paper.

Theoretical Consideration and Basic Assumptions

The tidal prism concept has been used to evaluate the ability of an estuary to disperse pollutants[2,3]. The tidal prism is equal to the difference between water volumes at high and low tides. In an estuary, part of this volume is contributed by river flow, part by water which enters through the seaward boundary on the flooding tide. In a small coastal basin, the contribution of river water may be so small at times that the tidal prism consists wholly of the water brought in by the tide. This inter-tidal volume of water serves to dilute the introduced pollutants and eventually flushes them out of the estuary or coastal basin.

The objective of this model is to calculate the equilibrium distribution of introduced pollutants. During each tidal cycle, the pollutant concentration at any location varies with the stage of the tide, but on successively similar tidal stages, the pollutant concentration returns to the same value. For the equilibrium condition to exist, the pollutant discharge rates and river flow, if any, must be kept constant for a period much longer than the flushing time of the water body.

Ketchum's[3] assumption of the tidal prism concept is adapted with modification. Ketchum assumed complete mixing of the water entering on flood tide with all of the water present throughout the estuary at low tide. He further assumed that the maximum length of the estuary over which complete mixing is possible is determined by the average excursion of a water particle on the flood tide. In the present model, Ketchum's second assumption is retained and the water body is divided into segments of length equal to the local tidal excursion. Instead of complete mixing with all water present at low tide, the water entering on flood tide is assumed to mix completely with the water present in the most seaward segment at low tide. Some portion of this mixture, in turn, enters the next landward segment and mixes completely with the water present there at low tide. This process progresses landward until the limit of the estuary or coastal basin. On the ebb tide, the part of water making up the local inter-tidal volume of each segment escapes to the adjacent seaward segment. The flushing is thus accomplished by a series of tidal exchanges with the pollutants moving progressively seaward.

Segmentation

For the purpose of model construction, a water body is divided into segments each having a length equal to the local tidal excursion. In a small coastal basin, the critical time for water quality is usually at the period when the freshwater input is at a minimum, or zero. The method of segmentation employed by Ketchum cannot be applied because it requires the river flow as a non-zero parameter to start the segmentation process from the head of the estuary. In the present model, the segmentation process starts from the mouth of the water body and the length of each segment is chosen to equal the tidal excursion with zero freshwater inflow.

Figure 1 shows the plain view of a coastal basin with its volume $V(x)$ and tidal prism $P(x)$ plotted as function of distance x from the mouth. $V(x)$ is defined as the accumulated low-tide volume along the main stem from the mouth to the transect at x. P(x) is the inter-tidal volume landward from the transect at x, including those of branches. The most seaward segment (segment no. 1) is defined between transects 1 and 2 such that its low-tide volume V_1 equals to the tidal prism landward of transect 2, i.e. P_2. In general,

$$\begin{aligned} V_n &= P_{n+1} \\ &= P_{n+2} + p_{n+1} \\ &= V_{n+1} + p_{n+1} \end{aligned} \qquad (1)$$

where V_n is the low-tide volume of the nth segment which is between the nth and (n+1)th transects, P_{n+1} is the tidal prism landward from the (n+1)th transect and p_{n+1} is the local tidal prism, or inter-tidal volume of the (n+1)th segment. Therefore, the low-tide volume of a segment equals the tidal prism landward from it and also it is equal to the high-tide volume of its adjacent landward segment.

The low-tide volume of a segment decreases monotonically landward as the tidal prism decreases. If the basin has a vertical shoreline, then in principle, $V_n \to 0$ as $n \to \infty$ and there will be an infinite number of segments. Complete mixing is never achieved at the landward end of the basin because of the diminishing tidal excursion. If the basin has a sloping beach, the volume of the most landward segment may be chosen as the tidal prism of those areas which are exposed at low tide and submerged at high tide.

Each of the branches of the basin may be segmented in the same way as that of the main stem.

Distribution of Conservative Pollutants

If one assumes that a conservative pollutant is discharged into the mth segment at a rate of Q per tide, the pollutant concentration in each segment may be calculated by considering the mass balance.

Segments Seaward of Outfall

Under equilibrium conditions, the net amount of the pollutant 'flushed' across a transect seaward of the outfall, i.e. $n \leq m$, must be equal to Q. A volume of water P_n is transported seaward and landward on ebb and flood tides respectively. Let C_n be the concentration of the nth segment at high tide, then the total mass transported seaward during ebb tide is P_nC_n. Since the flooding water is assumed to mix completely with the water present in the (n-1)th segment at low tide before it is transported across the nth transect, that water transported landward will have concentration C_{n-1}, the concentration of the (n-1)th segment at high tide. Therefore

$$P_nC_n - P_nC_{n-1} = Q, \text{ or}$$

$$C_n = C_{n-1} + \frac{Q}{P_n} \qquad \text{for } m \geq n \geq 1 \qquad (2)$$

Equation (2) requires that C_o be specified before the concentration distribution may be calculated. This is equivalent to the boundary condition requirement for solution of an advection-diffusion equation. Assuming that a fraction α of the water entering the basin through transect 1 on flood tide is water that escaped from the basin during the previous ebb tide, then

$$C_o = \alpha C_1$$

and equation (2) becomes

$$C_1 = \frac{Q}{(1-\alpha)P_1} \qquad \text{for } n = 1 \qquad (3)$$

In general, equation (2) becomes

$$C_n = \frac{Q}{(1-\alpha)P_1} + \sum_{i=2}^{n} \frac{Q}{P_i} \qquad (4)$$

If a flushing rate γ_n is defined as the portion of the pollutant removed from the nth segment per tidal cycle, mass balance requires that

$$\gamma_nC_n\ (V_n + p_n) = Q$$

where $C_n\ (V_n + p_n)$ is the total mass of the pollutant in the nth segment at high tide. Then

$$\begin{aligned} \gamma_n &= \frac{Q}{(V_n + p_n)C_n} \\ &= \frac{1}{(V_n+p_n)\left(\frac{1}{(1-\alpha)P_1} + \sum_{i=2}^{n} \frac{1}{P_i}\right)} \end{aligned} \qquad (5)$$

Segment Landward of Outfall

If the nth segment is located landward from the outfall, calculation of the pollutant concentration may be considered an intrusion problem. Under equilibrium conditions, there should be no net transport of the pollutant across the nth transect, thus

$$P_nC_n - P_nC_{n-1} = 0$$

$$C_n = C_{n-1}$$

In general,

$$C_n = C_m \qquad \text{if } n \geq m \qquad (6)$$

Distribution of Nonconservative Pollutants

In addition to flushing by tidal action, a nonconservative pollutant will undergo a decaying process which will further reduce the concentration distribution in a water body. The mechanisms of tidal flushing and decay may be assumed to work independently and their combined effect may be studied through the principle of mass-balance in a segment of the basin.

If W_n is the total mass of the pollutant in the nth segment, then the amount of the pollutant removed per tidal cycle by tidal flushing is γ_nW_n, where γ_n is the flushing rate defined previously. The remaining mass of the pollutant $(1-\gamma_n)W_n$ will undergo decay. Assuming that the pollutant decays linearly with a decay rate of k per tide, the amount of the pollutant decaying in one tidal cycle will be $(1-\gamma_n)\ W_n(1-e^{-k})$. Therefore, the total loss of the pollutant per tidal cycle is

$$\gamma_n W_n + (1-\gamma_n) W_n (1-e^{-k}) = \left(1-(1-\gamma_n)e^{-k}\right) W_n$$

Under equilibrium conditions, the same amount of the pollutant has to be supplied by the adjacent segment closer to the pollutant source, thus,

$$\left(1-(1-\gamma_n)e^{-k}\right) W_n = \gamma_{n+1} W_{n+1}$$

or

$$W_n = \frac{\gamma_{n+1} W_{n+1}}{1-(1-\gamma_n)\, e^{-k}} \qquad (7)$$

If the pollutant were not decaying during the time it is transported from the (n+1)th segment to the nth segment, equation (7) might be reduced to

$$(W_n)_o = \frac{\gamma_{n+1}}{\gamma_n} W_{n+1} \qquad (8)$$

where $(W_n)_o$ is the total mass of the pollutant in the nth segment with no decay in the segment. By combining equations (7) and (8), the following is obtained

$$W_n = \frac{\gamma_n}{1-(1-\gamma_n)e^{-k}} (W_n)_o \qquad (9)$$

Equation (9) states that the factor for pollutant reduction due to decay within the nth segment is

$$\frac{\gamma_n}{1-\ (1-\gamma_n)\ e^{-k}}$$

which also has been shown independently by Ketchum, et al.[4]. Equations (4) and (6) give the concentration distribution due to the flushing by tidal action alone. After applying the decaying factor, the concentration distribution of a nonconservative pollutant may be summarized as follows:

$$C_n = \prod_{i=n}^{m} \frac{\gamma_i}{1-\ (1-\gamma_i)e^{-k}} (C_n)_o \quad \text{if } n \leq m \qquad (10)$$

and

$$C_n = \prod_{i=m}^{n} \frac{\gamma_i}{1-\ (1-\gamma_i)\ e^{-k}} (C_n)_o \quad \text{if } n>m \qquad (11)$$

where $(C_n)_o$ is the concentration of a conservative pollutant and is given by equation (4) or (6).

If the decay rate is zero, equations (10) and (11) reduce to $C_n = (C_n)_o$. It is apparent that for any given flushing rate, any increase in the decay rate will decrease the concentration. However for a pollutant with a given decay rate, a larger flushing rate will result in higher relative concentrations compared to those of the conservative pollutant, since the pollutant remains within the segment of the water body for a shorter time.

Model Application

The model has been applied to the Cockrell Creek, Virginia, a small coastal basin located near the mouth of the Great Wicomico River, which itself is a tributary of the Chesapeake Bay. The creek is about 3.5 miles (5.63 km) long with a width ranging from 300 ft. (91.5m) to 1300 ft. (396m). The total drainage area is 4.6 mi^2 (11.9 km^2). Examination of the salinity distribution (figure 2) reveals that at times in the summer the creek is well-mixed and the freshwater inflow is almost zero. This condition makes the tidal prism concept most applicable.

A 0.2 MGD (0.0088 m^3/S) sewage treatment plant was proposed for the treatment of the sewage from the town of Reedville and two nearby fish processing plants. The primary environmental concern is the effect of the proposed waste discharge on the shellfish due to the possible increase of coliform bacteria and depletion of dissolved oxygen. The Food and Drug Administration has a water quality standard of 14 MPN/100 ml of fecal coliform for shellfish harvesting.

Figure 3 shows the segmentation of Cockrell Creek according to the tidal prism concept. The tidal prisms, low-tide volumes and flushing rates are listed in Table 1. Two sets of flushing rates were calculated, with $\alpha = 0$ and 0.5 respectively, where α is the fraction of the water entering the creek at flood tide which left the creek during the previous ebb tide. It is preferable that α be determined by a tracer experiment in the prototype. However, the data in the table show that the dependence of flushing rates on the value of α diminishes rapidly in the landward direction. For example, a change of α from 0.0 to 0.5 changes the flushing rate at segment M5 by only 11%.

The model was used to calculate the fecal coliform and BOD (biochemical oxygen demand) concentrations in the creek. The proposed outfall is located in segment M5. The effluent is secondary treated sewage with 24 mg/l of BOD$_5$ and 200/100 ml of fecal coliform. Assuming a BOD decay rate of 0.1/tide and coliform die-off rate of 0.5/tide, the following concentrations for segments adjacent to the outfall were obtained with the flushing rates corresponding to $\alpha = 0.5$:

Segment	BOD mg/l	Fecal Coliform MPN/100 ml
M4	0.048	0.09
M5	0.078	0.25
M6	0.065	0.14
B1	0.070	0.17
C1	0.074	0.21

The above table shows that the increase in the fecal coliform count at segment M5 will be 0.25/100 ml if α is assumed to be 0.5. For a more conservative estimate, α is assumed to be 0.9, then the flushing rate and fecal coliform count at segment M5 will be 0.113/tide and 0.28/100 ml respectively. The low sensitivity of the coliform concentration in response to the value of α lies in the fact that the lower flushing rate allows a longer time for bacteria to die off in any particular segment.

Discussion

The tidal prism method of Ketchum has been modified and applied to small coastal basins with negligible freshwater runoff. Ketchum's method was designed for use in the estuaries where the freshwater may be treated as a tracer. In his method, the estuary is segmented from its head to mouth using both the river flow and tidal prism as parameters. The segmentation process fails in the singular case of zero freshwater inflow. The modified method proposed here uses the tidal prism as the sole parameter to segment a coastal basin from its mouth to head. The flushing rate of each segment

Table 1. Values of P_n, V_n, γ_n for the segments in the Cockrell Creek.

Segment or Transect	P_n (10^4 ft.^{3})	V_n (10^4 ft.^{3})	γ_n (1/tide)	
			α=0.0	α=0.5
M1	3810	3355	1.00	0.5
M2	3355	2920	0.53	0.36
A1	215	170	0.89	0.85
A2	170	120	0.53	0.52
A3	120	357	0.11	0.11
M3	2705	2317	0.40	0.31
M4	2317	2105	0.32	0.27
M5	2105	1799	0.26	0.23
B1	603	500	0.47	0.44
B11	136	105	0.68	0.66
B12	105	255	0.14	0.14
B2	364	296	0.44	0.42
B21	60	156	0.25	0.25
B3	236	180	0.40	0.39
B31	84	192	0.16	0.16
B4	96	359	0.11	0.11
C1	246	200	0.69	0.66
C2	200	155	0.46	0.45
C3	155	122	0.37	0.37
C4	122	313	0.09	0.09
M6	950	787	0.37	0.33
D1	62	138	0.26	0.26
M7	725	600	0.32	0.31
M8	600	493	0.28	0.27
E1	93	196	0.21	0.21
M9	400	280	0.30	0.29
M10	280	200	0.30	0.29
M11	200	150	0.29	0.29
M12	150	100	0.28	0.28
M13	100	60	0.30	0.30
M14	60	60	0.17	0.17

was derived from a more rigorous mass-balance principle instead of intuitively defining it as the ratio of intertidal volume to segment volume.

The proposed model is most practical for environmental studies for a small project in a small coastal basin. In the absence of freshwater runoff, the small coastal basins tend to be well-mixed and the tidal exchange is the sole mechanism to flush out the pollutant. The method requires a minimum amount of data: the tidal range and the volume of the basin. The only parameter which needs to be calibrated is the returning ratio α, the fraction of water entering the basin at flood tide which left the basin during the previous ebb tide. This parameter may be determined by conducting tracer experiments in the prototype. However the dependence of the flushing rates on the value of α decreases rapidly as the segments proceed landwards. The predicted concentration distribution of a nonconservative pollutant is rather insensitive to the change in the value of α.

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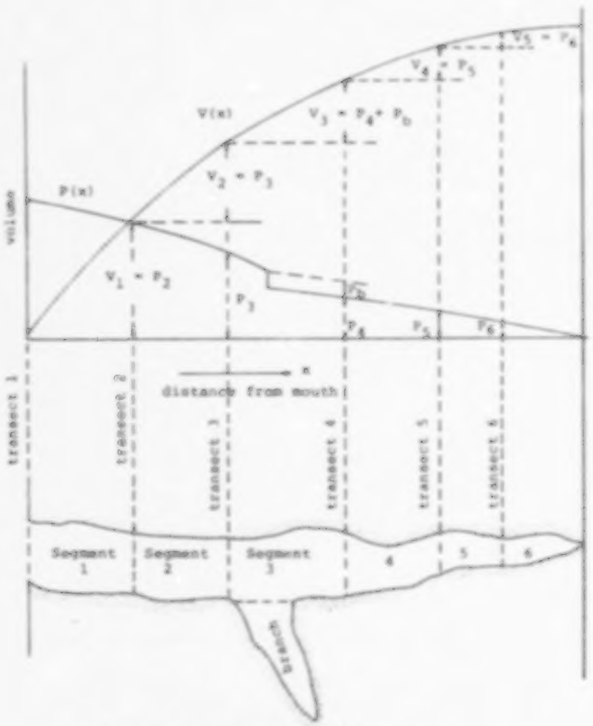
V(x)
P(x)
volume
$V_1 = P_2$
$V_2 = P_3$
$V_3 = P_4 + P_b$
$V_4 = P_5$
$V_5 = P_6$
P_3
P_b
P_4
P_5
P_6
x
distance from mouth
transect 1
transect 2
transect 3
transect 4
transect 5
transect 6
Segment 1
Segment 2
Segment 3
4
5
6
branch

Segmentation Criterion: $V_n = P_{n+1} + P_b$
V_n = low-tide volume of the nth segment
P_{n+1} = tidal prism landward from the (n+1)th transect
P_b = tidal prism of the branch connecting to the segment

Figure 1. Segmentation of a Coastal Basin.

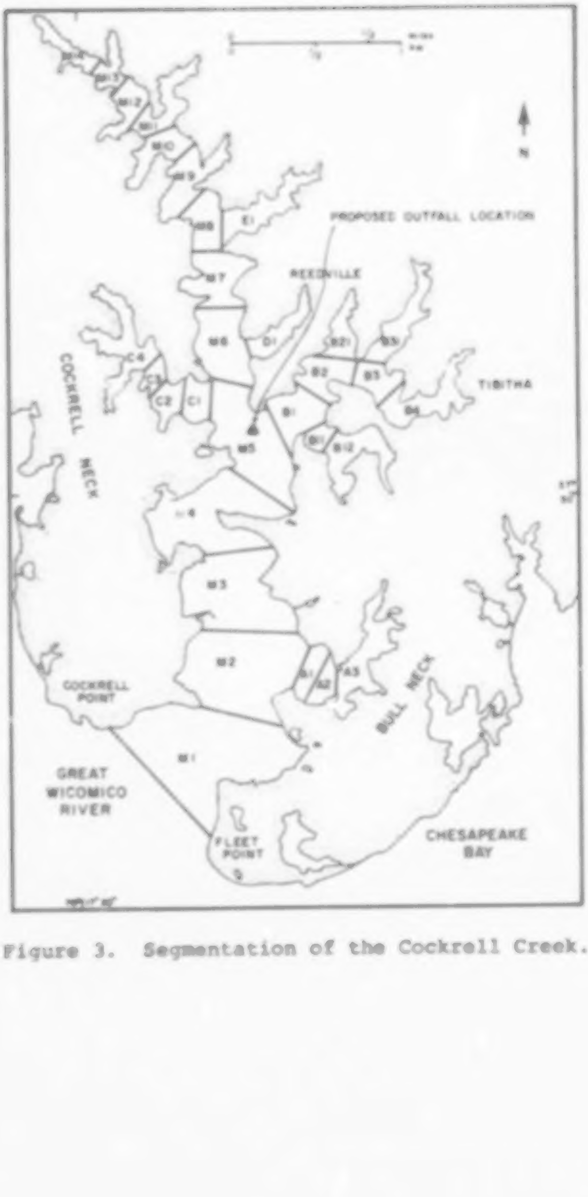
M14
M13
M12
M11
M10
M9
M8
E1
M7
M6
D1
B21
B3
B2
B3
B4
C4
C3
C2
C1
B1
B11
B12
M5
M4
M3
M2
A1
A2
A3
M1
N
PROPOSED OUTFALL LOCATION
REEDVILLE
TIBITHA
COCKRELL NECK
BULL NECK
COCKRELL POINT
GREAT WICOMICO RIVER
FLEET POINT
CHESAPEAKE BAY

Figure 3. Segmentation of the Cockrell Creek.

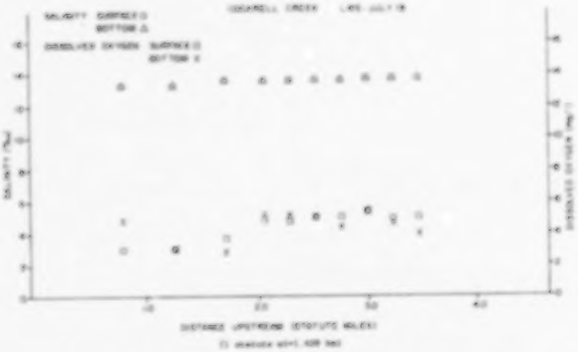

Figure 2. Longitudinal Salinity Distribution in the Cockrell Creek, Virginia.

EVALUATION OF MATHEMATICAL MODELS
FOR THE SIMULATION OF TIME-VARYING RUNOFF AND WATER QUALITY
IN STORM AND COMBINED SEWERAGE SYSTEMS

Albin Brandstetter
Research Associate
Water and Land Resources Department
Battelle - Pacific Northwest Laboratories
Richland, Washington

Richard Field
Chief
Storm and Combined Sewer Section
Municipal Environmental Research Laboratory
U. S. Environmental Protection Agency
Edison, New Jersey

Harry C. Torno
Staff Engineer
Media Quality Management Division
Office of Research and Development
U. S. Environmental Protection Agency
Washington, D. C.

ABSTRACT

The use of mathematical models for the assessment, planning, design, and control of storm and combined sewerage systems is becoming wide-spread in order to develop more cost-effective wastewater management schemes than are possible with conventional steady-state analysis techniques. The U.S. Environmental Protection Agency has sponsored an assessment of simulation models to provide a readily available reference guide for selecting models best suited for specific purposes. Most models reviewed include the computation of the time-varying runoff from rainfall and flow routing in sewerage networks. Some models simulate the time-varying wastewater quality, and a few models include mathematical optimization techniques for the least-cost design of new sewer system components or for optimal real-time operation of combined sewer overflow structures. The assessment summarized the principal features, assumptions and limitations of each model and compared numerical test results and computer running costs for seven models. Additional model features were recommended which would enhance or extend model simulation capabilities and use.

INTRODUCTION

Mathematical models are being used more frequently for the assessment of existing sewerage system performance, the planning and design of new facilities, and the control of untreated overflows during rainstorms. For some purposes, primarily the design of sanitary sewerage systems, steady-state models are adequate to compute the least-cost combinations of sewer pipes and slopes for specified inflows. Nonsteady-state models are required, however, to adequately analyse complex storm and combined sewerage systems under dynamic runoff conditions.

A considerable number of steady-state and nonsteady-state models have been developed in the last few years for the analysis of sewerage systems. It is consequently becoming increasingly confusing for the user to select the model most suited for a particular application. A review of the more comprehensive nonsteady-state urban hydrologic models was therefore conducted to develop a brief summary of most available models and to provide a reference of model features and their strengths and limitations.[1]

MODEL COMPARISONS

The following models were reviewed (models marked with * were also tested with computer runs):

*1. Battelle Urban Wastewater Management Model[2,3]
2. British Road Research Laboratory Model[4,5]
*3. Chicago Flow Simulation Program[6,7]
4. Chicago Hydrograph Method[8,9] and Runoff and Pollution Models[10]
5. CH2M-Hill Wastewater Collection System Analysis Model[11]
6. Colorado State University Urban Runoff Models[12,13,14]
7. Corps of Engineers STORM Model[15,16]
*8. Dorsch Consult Hydrograph-Volume Method[17] and Quantity-Quality Simulation Program[18]
*9. Environmental Protection Agency Storm Water Management Model[19,20]
10. Hydrocomp Simulation Program[21,22]
11. Illinois State Water Survey Urban Drainage Simulator[23]
*12. Massachusetts Institute of Technology Urban Watershed Model[24,25]
13. Minneapolis-St. Paul Urban Runoff Model[26]
14. Norwegian Institute for Water Research Sewerage System Models[27]
15. Queen's University Urban Runoff Model[28]
16. Seattle Computer Augmented Treatment and Disposal System[29]
*17. SOGREAH Looped Sewer Model[30]
18. University of Cincinnati Urban Runoff Model[31]
19. University of Illinois Storm Sewer System Simulation Model[32,33]
20. University of Massachusetts Combined Sewer Control Simulation Model[34]
21. University of Nebraska Urban Hydrologic Simulator[35]
22. Watermation Cleveland Sewer Model[1]
*23. Water Resources Engineers Storm Water Management Model[36]
24. Wilsey and Ham Urban Watershed Model[37]

In general, the reviewed models combine the runoff from several catchments and route the wastewaters within the sewer networks. Most of them consider the spatial nonuniformity of rainfall; the time-varying runoff resulting from rainstorms of different intensities and durations; spatial and temporal variations in dry-weather flows; the attenuation of flows during overland, gutter, and sewer conduit flow routing; and

Table 1. COMPARISON OF MAJOR MODEL CATEGORIES

	MODEL ORIGIN	MODEL ABBREVIATION	YEAR	CATCHMENT HYDROLOGY							SEWER HYDRAULICS								WASTEWATER QUALITY									MISCELLANEOUS					
				MULTIPLE CATCHMENT INFLOWS	DRY-WEATHER FLOW	INPUT OF SEVERAL HYDROGRAPHS	SNOWMELT	RUNOFF FROM IMPERVIOUS AREAS	RUNOFF FROM PERVIOUS AREAS	WATER BALANCE BETWEEN STORMS	FLOW ROUTING IN SEWERS	UPSTR AND DOWNSTR FLOW CONTROL	SURCHARGING AND PRESSURE FLOW	DIVERSIONS	PUMPING STATION	STORAGE	PRINTS STAGE	PRINTS VELOCITIES	DRY-WEATHER QUALITY	STORMWATER QUALITY	QUALITY ROUTING	SEDIMENTATION AND SCOUR	QUALITY REACTIONS	WASTEWATER TREATMENT	QUALITY BALANCE BETWEEN STORMS	RECEIVING WATER FLOW SIMULATION	RECEIVING WATER QUALITY SIMULATION	CONTINUOUS SIMULATION	CAN CHOOSE TIME INTERVAL	DESIGN COMPUTATIONS	REAL-TIME CONTROL	APPLIED TO REAL PROBLEMS	COMPUTER PROGRAM AVAILABLE
1	BATTELLE NORTHWEST	BNW	1975	●	●	●		●	●		●		●	●		●	●	●	●	●	●			●					●	●	●	●	●
2	BRITISH ROAD RESEARCH LAB	RRL	[illegible]	●	●	●		●			●															●			●			●	●
3	CHICAGO SANITARY DISTRICT	FSP	1976	●	●	●	●	●	●	●	●					●	●									●		●	●			●	●
4	CH2M-HILL	SAM	1976	●	●	●		●	●	●	●		●	●	●		●												●				
5	CITY OF CHICAGO	CHI-HYD	1976	●	●	●		●	●	●	●		●	●				●	●	●				●		●		●	●	●		●	●
6	COLORADO STATE UNIVERSITY		1976	●	●			●			●	●					●	●															●
7	CORPS OF ENGINEERS	STORM	1976				●	●	●	●				●		●				●			●		●			●				●	●
8	DORSCH CONSULT	HVM-QQS	1975	●	●	●		●	●	●	●	●	●	●		●	●	●	●	●	●		●	●	●	●	●		●			●	
9	ENV. PROTECTION AGENCY	SWMM	1976	●	●	●		●	●		●	●	●	●	●	●			●	●	●	●	●	●		●	●		●	●		●	●
10	HYDROCOMP	HSP	1976	●	●	●	●	●	●	●	●	●		●		●	●	●	●	●	●		●		●	●	●	●	●		●	●	
11	ILLINOIS STATE	ILLUDAS	1976	●	●	●		●	●		●					●	●												●	●			●
12	MIT-RESOURCE ANALYSIS	MITCAT	1972	●	●	●	●	●	●		●		●	●		●	●	●								●			●			●	
13	MINNEAPOLIS-ST. PAUL	[illegible]	1971	●	●	●		●	●		●			●															●		●	●	●
14	NORWEGIAN WATER RES.	NIVA	1976	●	●						●	●	●	●	●	●			●	●	●			●				●	●	●			
15	QUEEN'S UNIVERSITY	QUURM	1975	●				●	●		●																						
16	SEATTLE METRO	CATAD	1976	●	●	●		●	●	●	●	●	●	●	●	●	●												●		●	●	●
17	SOGREAH	CAREDAS	1976	●	●			●	●		●	●	●	●	●	●	●	●			●					●	●		●			●	
18	UNIVERSITY OF CINCINNATI	UCUR	1976	●				●	●		●															●			●				●
19	UNIVERSITY OF ILLINOIS	ISS	1975	●	●		●	●	●		●	●		●	●	●	●	●											●	●			●
20	UNIVERSITY OF MASSACHUSETTS		1976	●	●			●		●	●	●					●	●										●					●
21	UNIVERSITY OF NEBRASKA	[illegible]	1976	●		●		●	●		●																		●				
22	WATERMATION	[illegible]	1975	●	●	●		●	●		●	●	●	●	●	●	●	●	●	●	●			●					●	●	●	●	
23	WATER RESOURCES ENGINEERS	STORMSEWER	1975	●	●	●		●	●		●	●	●	●	●	●	●	●	●	●	●		●			●	●		●			●	
24	WILSEY AND HAM	WH-1	1972	●				●	●		●																		●	●		●	

the operation of flow diversion structures and storage facilities under dynamic wastewater flow conditions. Only a few models exist, however, which also compute the water quality of the urban runoff and route the pollutants through the sewerage networks. Some models include options for dimensioning sewer pipes and two of them use mathematical optimization schemes for least-cost design of new sewerage system components. Three models have provisions for the real-time control of overflows during rainstorms.

Table 1 lists the principal features of the models. Detailed model descriptions and comparison tables, results of numerical testing for 7 models, and recommendations for future model improvements are contained in the project report submitted to the U.S. Environmental Protection Agency.[1]

A brief review of these models indicates a tremendous diversity in scope and purpose, mathematical detail, system elements and hydrologic phenomena being modeled, size of the system that can be handled, data input requirements, and computer output. This diversity, of course, is a result of the varying conditions and objectives which govern the design and evaluation of individual sewerage systems, limitations in the available computer hardware, and progress in the state-of-the-art of modeling specific phenomena.

For some applications, models are available with considerable simplifications in their mathematical detail to reduce input data requirements, computer storage requirements, and computer running time. Some models include unnecessary approximations considering the present state-of-the-art of hydrologic modeling and computer capability. Some of the simplifications, however, are needed for applications to real-time control of overflows which require repeated simulations within fixed time constraints on a small process computer.

Usually the simplest model which simulates the desired phenomena with adequately accurate mathematical formulations should be selected. Input data requirements and computer running times generally decrease with decreasing complexity of the model. Some models include options to suppress portions of the simulation if only selected phenomena are of interest. Although this feature is not listed, it should be considered in the model selection. Some proprietary models have features which appear superior to the publicly available models, but a user may prefer to run his own model that does not exactly meet his requirements.

The simulation of water quality adds considerable complexity to a model, even if it routes only conservative substances. The complexity increases substantially if both storm and dry-weather water quality is computed from land use characteristics. Additional complexities are added if wastewater treatment and receiving water flow and quality are being modeled.

The testing and review of the models indicated also that the routing of flow and conservative pollutants, although complex for looping and converging and diverging branch systems with special structures, are the best understood phenomena. The selection of particular mathematical formulations and numerical solution techniques is governed only by the preference and needs of the model developer and user. Research is required, however, to provide a better understanding of sedimentation and scour, and of reactions and interactions between various pollutants in the sewers.

Considerable uncertainties exist in the modeling of catchment phenomena, both the flow and water quality of storm and dry-weather runoff. The definition of adequate formulations for soil infiltration, the filling of depression storage, evapotranspiration, groundwater seepage and soil moisture are extremely difficult considering the heterogeneity of catchment land uses, geometry, vegetation, and soils. The adequacy of catchment water quality computations from catchment land use and runoff has not been sufficiently demonstrated. Although various models have shown good agreement between measured and computed catchment runoff water quality, the comparisons have been too limited to assign confidence limits to predictions for catchments without measurements. The models are still useful, however, for the evaluation of relative merits of alternative wastewater management schemes.

In general, a direct relationship between model complexity and its cost of implementation and application exists with respect to the number of major phenomena which are modeled. Efficient solution algorithms, however, may reduce this difference significantly. This is true particularly for proprietary models due to their need to stay competitive. A model which simulates many special sewerage system facilities will be more complex in structure and require more data and computer storage than a model that computes only runoff from a single catchment without routing flows or which routes only flow in a simple converging network without computing runoff from precipitation and land use.

Model testing with hypothetical data showed that computer running time of models simulating the same phenomena is governed more by efficient formulations of the overall model logic than by the basic equations used for specific phenomena. For instance, no consistent pattern in computer running time was evident between the use of the kinematic and dynamic wave equation. Consequently, since the dynamic wave equation can be solved to simulate downstream flow control, backwater, flow reversal, surcharging, and pressure flow (none of which can be simulated by the kinematic wave equation) the application of models using the dynamic wave equation is recommended, provided the selected model includes an efficient numerical algorithm for its solution.

Some models require only the input of typical subcatchment elements and perform hydrologic computations only for these typical subcatchments, but then consider the actual locations of all subcatchments for the overland and sewer flow routing computations. This can save considerable input preparation and computer running time.

RECOMMENDATIONS

Various models stand out due to their completeness of hydrologic and hydraulic formulations, the ease of input data preparation, the efficiency of computational algorithms, and the adequacy of the program output. Other models, although deficient in some of these respects, merit consideration due to special features which are not included in the more comprehensive models but may be required for specific applications.

The following models are consequently recommended for routine applications:

1. Battelle Urban Wastewater Management Model for real-time control and/or design optimization considering hydraulic, water quality and cost constraints, provided the hydrologic and hydraulic model assumptions are adequate for particular applications (lumping of many small subcatchments into few large catchments, neglect of downstream flow control, backwater, flow reversal, surcharging, and pressure flow).

2. Corps of Engineers STORM Model for preliminary planning of required storage and treatment capacity for storm runoff from single major catchments, considering both the quantity and quality of the surface runoff and untreated overflows.

3. Dorsch Consult Hydrograph Volume Method for single-event flow analysis considering most important hydraulic phenomena (except flow reversal). A Quantity-Quality Simulation Program for continuous wastewater flow and quality analysis is now available, but the model was completed too late for evaluation.

4. Environmental Protection Agency Stormwater Management Model for single-event wastewater flow and quality analysis provided the hydraulic limitations of the model are acceptable (neglect of downstream flow control and flow reversal, inadequate backwater, surcharging, and pressure flow formulation). A new version patterned after the Corps of Engineers STORM Model is now available for continuous simulation, but this version was completed too late for evaluation.

5. Hydrocomp Simulation Program for single-event and continuous wastewater flow and quality analysis provided the hydraulic limitations of the model are acceptable (approximate backwater and downstream flow control formulation, neglect of flow reversal, surcharging, and pressure flow).

6. Massachusetts Institute of Technology Urban Watershed Model for single-event flow analysis provided the hydraulic limitations of the model (neglect of backwater, downstream flow control, backwater, flow reversal, surcharging, and pressure flow), or the use of a separate model for these phenomena is acceptable.

7. Seattle Computer Augmented Treatment and Disposal System as an example of an operating real-time control system to reduce untreated overflows. A more comprehensive computer model simulating both wastewater flow and quality and including mathematical optimization should be considered, however, for new systems.

8. SOGREAH Looped Sewer Model for single-event wastewater flow and quality analysis considering all important hydraulic phenomena.

9. Water Resources Engineers Stormwater Management Model for single-event wastewater flow and quality analysis considering all important hydraulic phenomena.

The remaining reviewed models do not appear to provide sufficient special features which are not included in the models mentioned above. Their use may be advantageous, nevertheless, for certain applications where model assumptions are adequate, and especially where assistance from the model developers is easily available.

SUMMARY

In general, the reviewed models provide useful tools to the engineer and planner for assessing, designing, planning and controlling storm and combined sewerage systems. It is extremely important, however, that the potential model user study the formulations of the models, their limitations and approximations, if he is to use the models in an appropriate manner. In addition, discussions with both the original model developers and other model users can provide significant information with respect to new model features and use experience not found in published reports.

ACKNOWLEDGMENTS

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USE OF MATHEMATICAL MODELS FOR HYDROLOGIC FORECASTING IN THE NATIONAL WEATHER SERVICE

John C. Schaake, Jr.
Assistant Director
Hydrologic Research Laboratory
National Weather Service
National Oceanic and Atmospheric Administration
Silver Spring, Maryland

ABSTRACT

The National Weather Service is implementing a new system of mathematical models to aid river forecasters throughout the United States. Forecasts of stages and discharges a few days ahead are produced routinely on a daily basis and at six-hour intervals during floods. Also, extended streamflow prediction of high, low, and expected discharges for periods up to several months into the future are made at routine intervals.

This system of models, known as the "National Weather Service River Forecast System" (NWSRFS), was initiated in 1971[9] and is now being improved and expanded. It includes conceptual hydrologic models of snow, soil moisture, and streamflow routing; it includes models of unsteady open channel flow; it has provisions for reservoir operations models; and it will include stochastic hydrometeorologic models to account for uncertainty in streamflow forecasts. NWSRFS also includes programs and procedures for model calibration and verification with the historical data. Studies of the validity and accuracy of the models are reviewed, and some modeling issues in need of further study are summarized.

Information generated by these models could contribute to EPA's overall environmental mission. Hydrologic information is readily available in NWS forecast data files for use with convection and dispersion models to forecast the fate of pollutants suddenly released to the hydrologic environment or to forecast the day to day variations in pollutant transport properties of selected streams. Currently under development is a water temperature forecast model utilizing hydrological and meteorological data readily available in real time in NWS data files.

Problems faced by NWS managers in understanding and utilizing NWSRFS are discussed. NWSRFS is being installed on an IBM 360/195* in Suitland, Md., and is being operated from remote terminals by field offices. NWSRFS is developed and supported by the Hydrologic Research Laboratory, Hydrologic Services Division, and the field offices.

HISTORY OF MODEL USE IN NWS

For many years, river forecasts in the U.S. have been made using an Antecedent Precipitation Index (API) type of rainfall-runoff relation to convert rainfall into rainfall excess or runoff.[7] Unit hydrographs or time delay histograms have been widely used to translate runoff through catchments to forecast points. These techniques historically have worked well and are still in use.

In 1966 a project was initiated in NWS to evaluate newly developed hydrologic models. Models were compared for a group of seven carefully selected basins throughout the country. No single numerical scoring factor seemed adequately to represent model accuracy because important differences between models seemed to be evident only in one or two aspects of the simulation or only in certain hydrologic situations. Several statistical measures based on observed and simulated discharge were used to evaluate model performance. Two models showed an accuracy advantage over API. One was essentially the same as the Stanford Watershed Model IV,[3] the other was the initial version of the Sacramento River Forecast Center Hydrologic Model.[2]

The most notable accuracy advantage of these conceptual models over the API model is during and after a long dry spell. The more complete moisture accounting techniques give the conceptual models enough "memory" to handle situations where large amounts of rain give little or no streamflow response.

In 1971 a modified version of the Stanford IV model was incorporated with other data processing programs into the NWSRFS.[11] A snow accumulation and ablation model was added to NWSRFS in 1973. This snow model accounts in detail for the energy balance of the snow cover by using air temperature to estimate energy exchanges.

The Hydrologic Research Laboratory in 1974 compared an improved Sacramento Model with the NWSRFS Stanford Watershed Model IV. Data from four catchments were used to test model performance. This was part of a WMO project on intercomparison of conceptual models. In general we concluded: (1) there is no significant difference in model performance in very humid areas; (2) there seems to be little difference in ability to simulate large flood events; (3) the Sacramento Model does simulate monthly volumes and small runoff events significantly better in semi-arid and moderately humid areas; and (4) improvements through research seemed easier to make to the Sacramento Model because of its modular structure. Following these model tests, components of the soil moisture accounting of the Sacramento Model replaced the original Stanford IV components in NWSRFS.

Summary of NWSRFS

NWSRFS includes techniques and programs for developing operational river forecasts from initial processing of historical data during procedure development to the preparation of forecasts in real time. The programs are generalized for use on any river system including headwater catchments and downstream river networks.

*Trade names are mentioned solely for purposes of identification. No endorsement by the NWS, NOAA, or Department of Commerce, either implicitly or explicitly, is implied.

Programs and example data sets for the initial version are available to the public through the National Technical Information Service (NTIS). Information to purchase these from NTIS can be obtained from the Hydrologic Research Laboratory (W23), National Weather Service, Silver Spring, Maryland 20910.

The following techniques and models are included in NWSRFS:

- Mathematical model of the accumulation and ablation of Snow [Anderson, 1973]
- A catchment model including both (a) a soil moisture model to account for flow through and above the soil mantle and for evapotranspiration and (b) time delay models to move runoff from the soil moisture model through the catchment to the catchment outlet
- Channel routing models to account for movement of water in a channel system
- Techniques for modeling the areal distribution precipitation
- Techniques for estimating mean areal temperature
- Methods to estimate model parameters using historical hydrometeorological data

CRITERIA FOR MODEL SELECTION

Some of the criteria we used for model selection are:

- Input Data Sampling Interval - Operational rainfall data are available from a 6-hour reporting network and a 24-hour reporting network. With this 6-hour reporting interval there is a lower limit to the size of catchment that can adequately be modeled.
- Computational Efficiency - Models are operated for most of the country. Each day, computations are made for the next few days using 6 hour time steps. During flood periods, computations are repeated every 6 hours.
- Data Availability - Historical hydrometeorological data are available in digital form for model calibration (i.e., model parameter estimation). Four types of data are available: (a) hourly precipitation data from the National Climate Center (NCC), Asheville, North Carolina (card deck 488); (b) daily observation data (NCC card deck 486); (c) synoptic meteorological data for estimating potential evaporation (NCC card decks 144, 345, and 480); (d) USGS daily streamflow data. All of these data for the period of digital record are available to NWSRFS users from a tape library of about 500 tapes at the NOAA computer center in Suitland, Maryland. Each of the tapes except streamflow is in a special format (O/H format) developed for the NWS Office of Hydrology (copies of tapes in this format are available to the public from NCC). Another main source of data are USGS topographic maps. (We generally use 1:250,000 scale maps.)
- Physical Validity - Within constraints imposed by computational efficiency and data availability, models should have physical basis for their structure and should simulate observed behavior reasonably well. Although models are usually compared by looking at differences between models, it is of interest to notice many models have some elements of common structure. This occurs because (a) water is held in storage as it flows through the hydrologic cycle and (b) rates of flow depend upon amounts of water in storage and possible other factors such as temperature, humidity, etc. Flow into and out of storage is governed by (a) a continuity relation and (b) a dynamic relation. Models differ in terms of spatial and temporal resolution of these relations and in terms of the factors accounted for in the dynamic relations.
- Building Block Structure - Models of individual processes (precipitation, evaporation, snow cover, soil moisture, channel routing, etc.) have been organized as building blocks. This offers flexibility to represent particular situations with varying degrees of physical detail, and it makes it possible for research on one phase of the hydrologic cycle to be evaluated in an environment that considers other phases.

Benefits Gained from these Criteria

Some of the benefits that accrue from these criteria, particularly the requirement for a strong physical base, are:

- Enhanced likelihood of adequately predicting future events especially during unexperienced hydrologic situations
- Potential to derive initial parameter values from streamflow records and from observable basin characteristics
- Parameters related to basin characteristics may possibly be adjusted without waiting for a new data base if basin characteristics change.
- Conceptual hydrologic models offer potential for application other than for forecasting river stage and discharge such as movement of pollutants through the environment, water temperature prediction, and prediction of soil moisture levels for agricultural purposes.

MODEL APPLICATIONS

Operational River Forecast Preparation

Daily river forecasts are prepared in 12 River Forecast Centers (RFC's) throughout the U.S. These RFC's transmit forecast information to Weather Service forecast offices (WSFO's) for dissemination to the public. The WSFO's gather precipitation and other data and transmit these to the RFC's.

There currently are about 6700 precipitation gages in our operational network. River stage data are gathered at least daily at 3100 locations. These data are used to prepare forecasts of river stage (and possibly discharge) at 2500 locations. Conceptual hydrologic models are now used at less than 10 percent of these forecast points.

Although the actual forecasts are made by professionals, not by computers, the computer is an essential tool in generating forecast information. A new operational forecast computer program currently is being developed under contract. This will be a disk-oriented system incorporating all of the NWSRFS hydrologic models and will be used from remote terminals by our RFC's. It will reside at the NOAA computer center in Suitland, Md. NOAA has 3 IBM 360/195 computers and these are used by NWS's National Meteorological Center (NMC) to operate its atmospheric simulation and forecast models and by the National Environmental Satellite Service (NESS) to operate two Geostationary Orbit Environmental Satellites (GOES). Additional current hydrologic and meteorological data from NWS and NESS operations are available or potentially available in various data files to our RFC's through this new operational forecast program.

The general configuration of our new operational program appears in Figure 1. Forecasters enter data as they become available from cards into time series files through a time series input routine. When a forecast is to be made, a preprocessing routine checks available data, estimates missing values, converts stages to discharges and computes mean areal precipitation, temperature, and potential evaporation. Then, the forecast routine reads the new mean areal time series data, the carry-over files from the previous forecast, and the model parameter data file. The forecast routine produces river forecasts and updates the carry-over files.

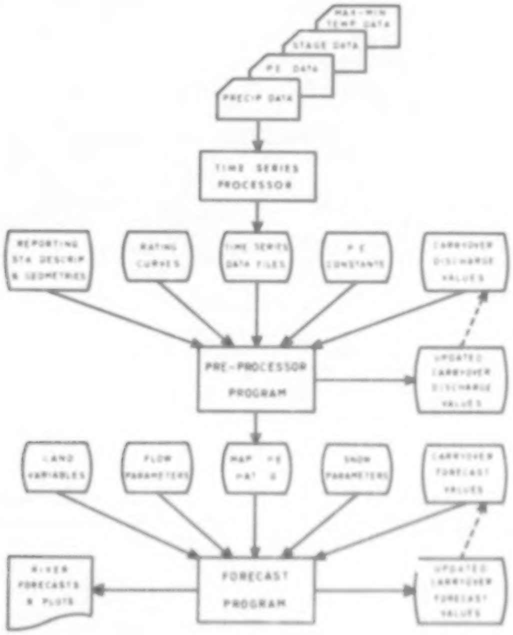

Figure 1. General Configuration of the NWS Operational Forecast Program

When new forecast points are added, model parameter values must be entered in the parameter data files and initial state variables must be entered in the carry-over files. The main problem, however, is to estimate the model parameters by analysis of historical data.

Parameter Estimation

To reduce the manpower costs of extending NWSRFS to the entire U.S. it would be nice to completely automate the parameter estimation process. However, it seems essential in mathematical optimization of parameters to start with good initial values and to constrain the domain of variation to avoid unrealistic estimates. This means some method other than automatic optimization is needed to analyze available information to find good initial values.

Our present approach is first to analyze historical precipitation and streamflow data to make initial estimates.[10] These are then used to simulate the system and results are analyzed to find possible adjustments. Finally, a pattern search[8] automatic optimization is used to "tune" the parameter estimates.

The most difficult part of our estimation procedure is to know how to make manual adjustments. Not only must one understand physically the dynamics of the natural process, but one must also understand mathematically the dynamics of the model of the process. There seems to be extremely strong tendencies for most professionals to rely only on their understanding of the physical process. We tend to assume how parameters should change rather than deduce this from our knowledge of the mathematics.

Historical Data Processing

Before parameter estimates can be made, historical data must be organized. We begin with a library of about 500 data tapes containing 4 different types of hydrometeorological data. We hope to add SCS snow course data in the near future to aid parameter estimation for our snow model. We also hope to add some USGS bi-hourly stage or discharge data. Data tapes are immediately available to our RFC's and we have programs to inventory individual tapes. We also have programs to strip selected time series and enter these into permanently mounted disk data files for future analysis. These disk files are part of our NWSRFS data file system. All of our data analysis and parameter estimation programs read and write time series using these files.

The initial version of NWSRFS was tape-oriented. All time series data, both measured and computed, were processed with magnetic tapes. This was extremely cumbersome because many intermediate tapes were required in preparation for model calibration. The direct access disk files in our current version greatly simplified our data handling problems.

Figure 2 illustrates the data processing options available to our RFC's to estimate parameters in our models. The inventory programs and preliminary processing programs strip data from tape to disk. The program MAP is used to convert raw precipitation data at hourly and daily stations into 6-hour mean areal values. Consistency checks are made via double mass plots of one station vs. any combination of other stations. Adjustments can be made in inconsistent data and missing data are estimated. Programs MAT and MAPE perform similar functions to produce mean areal temperature and potential evaporation data. Our manual calibration program, MCP, is used to simulate historical events using given parameter estimates. Our automatic optimization program uses direct search to find better parameter estimates.

Forecast Updating

Updating is needed in river forecasting because computed river stages up to the present time do not agree exactly with observed stages. Differences are due to errors in estimation of mean areal precipitation (our average precipitation gage density is only one gage per 450 square miles) and to modeling errors. In general improved forecasts can be made if

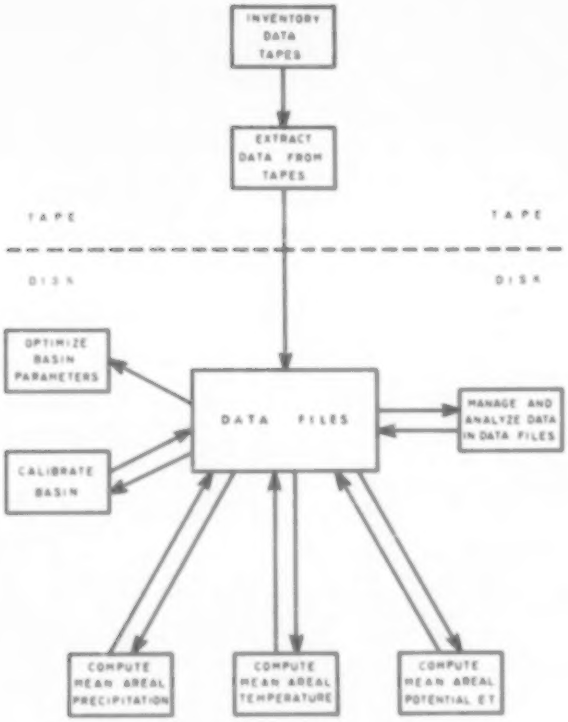
INVENTORY DATA TAPES
EXTRACT DATA FROM TAPES
TAPE
TAPE
DISK
DISK
OPTIMIZE BASIN PARAMETERS
CALIBRATE BASIN
DATA FILES
MANAGE AND ANALYZE DATA IN DATA FILES
COMPUTE MEAN AREAL PRECIPITATION
COMPUTE MEAN AREAL TEMPERATURE
COMPUTE MEAN AREAL POTENTIAL ET

Figure 2. Data Processing for Parameter Estimation in NWSRFS

differences between observed and computed stages are used to adjust forecast stages.

This can be done in several ways. One is to "blend" computed and observed stages directly by adding a proportion of the latest difference to the forecast. This proportion would decrease to zero into the future and the computed forecast would eventually prevail. A physically more attractive approach would be to adjust precipitation input data or unit hydrograph ordinates until observed and computed values agree within acceptable limits. Such adjustment procedures are now being studied by our Hydrologic Research Laboratory.

Mathematically, this updating problem arises whenever observations can be made of computed state variables. For example, we can observe snow water equivalent, extent of snow cover, soil moisture content, and ground water levels. Each is related in some way to model state variables. Unfortunately there is no general and practical way to use these additional data as input to conventional deterministic models. Perhaps a theoretical or conceptual framework can be derived from the Kalman filter in estimation theory. But this remains a difficult area of hydrologic research not only in river forecasting but wherever measurements of some output state variables are to be used to improve the estimates of other state variables.

POTENTIAL INTEREST TO EPA

Water is an important vehicle for transporting pollutants from point and non-point sources in the environment. Information on the current and forecast states of motion of water throughout the United States are continuously available in NWS data files.

Streamflow Routing

Potentially the streamflow routing models in NWSRFS could be of particular interest to EPA. We use several types of routing models ranging from unit hydrographs and time delay histograms to dynamic routing models based on the St. Venant partial differential equations for unsteady flow in open channels.

Unit hydrographs and time delay histograms are used currently to route runoff in headwater basins and local inflows to a downstream forecast point. Most widely used to route flow in streams and rivers is a "variable lag and K" method of accounting for the attenuation and delay of flood waves moving downstream. We currently are investigating possible use of Kinematic Wave and Diffusion Wave models in addition to these other models.

We have spent the last few years developing a dynamic routing model that would be computationally efficient and sufficiently accurate for operational forecasting.[4,5] We have a project underway to apply this model to the Mississippi and Ohio Rivers, including their junction.

Pollutant Transport Models

The potential exists for NWS or EPA to operate convection, dispersion, or other water quality models in conjunction with NWS models for such purposes as to forecast the fate of pollutants suddenly released into the environment, to aid in estimating the quantities of pollutants present (as opposed to concentrations), to forecast the day to day pollutant transport properties of selected streams, or to forecast quality changes in reservoirs.

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TESTING OF THE STORM WATER MANAGEMENT MODEL OF US EPA

Jiri Marsalek
Research Scientist
Hydraulics Research Division
Canada Centre for Inland Waters
Burlington, Ontario, Canada

SUMMARY

The results of testing the Storm Water Management Model (SWMM) on a number of urban test catchments are presented. The runoff quantity subroutine was tested and good results were obtained on eight catchments. The SWMM runoff quality subroutine was tested on three catchments only. The lack of data allowed only a qualitative discussion of the quality results obtained.

INTRODUCTION

Rapid advances in urban hydrology led to the development of a large number of urban runoff models in recent years, but only in the last three years have several comparative studies of various urban runoff models been undertaken to assist model users in model selection. Among these studies, the most notable were those sponsored by the Environmental Protection Agency[1] and the Canadian Department of Environment[10]. As a result of these studies, the Canadian Urban Drainage Subcommittee decided to adopt the SWMM model of US.EPA for further study, modification and application in urban runoff studies in Ontario. Some of the questions raised during this process were those of reliability of the SWMM model, the conditions under which the model could fail, and the accuracy of the SWMM simulations. All these questions are of utmost importance in planning and design of urban drainage systems.

When the SWMM model was developed, very little urban runoff data was available for model testing and verification. Consequently, only a limited testing of the model was carried out on four catchments and the limited data available allowed only a qualitative evaluation of the SWMM simulations[13]. Since then, several more extensive studies have been carried out on urban test catchments and the results were reported by Heeps and Mein[4], Jewell et al[5], Marsalek et al[6], Preul and Papadakis[9], and Shubinski and Roesner[11]. In all these cases, the number of test catchments was limited.

In this paper, the results of the SWMM model testing on a number of new test catchments are reported and a correlation between the accuracy of field observations and the accuracy of model simulations is demonstrated for runoff quantity.

METHODOLOGY FOR TESTING RUNOFF MODELS

When testing conceptual runoff models, the model tested is used to simulate the observed phenomena and the goodness of fit of the simulations to the observations is then evaluated. A set of criteria for evaluating the goodness of fit has to be devised and applied.

Modelling Errors

There is a number of sources of error causing the differences between the observations and simulations. These error sources include the following:

1. Bias in the simulated output (i.e. flows and their quality) because of incomplete or biased model structure.
2. Bias in the simulated output because of random or systematic errors in the input data (e.g. precipitation, catchment characteristics).
3. Random and systematic errors in the observed output (flows and their quality) used for comparisons with the simulated output.
4. Bias in the simulated output because of an incorrect application of the model (e.g. poor catchment discretization, selection of time steps, etc.).
5. Errors in the simulated output caused by an erroneous model calibration.

When testing conceptual models and their accuracy, it becomes extremely difficult to separate the effects of individual sources of error and to determine their contribution to the overall error. The last two errors, i.e. those caused by incorrect model application and calibration, can be significantly reduced and are eliminated here from further consideration. The errors due to uncertain input and output data (observations) are grouped here together and their effect on the accuracy of model simulations will be studied by statistical methods.

Selection of goodness of fit criteria

Runoff quantity. Numerous criteria of goodness of fit have been proposed for runoff models. For a review of some of these criteria, a reference is made to Fleming's work[2]. Fleming concluded, that no research has been undertaken to compare the various criteria available, and therefore, one can not define the best criteria for hydrologic modelling. He also suggested that the criteria should evaluate the following three parameters of a runoff hydrograph: the total runoff volume, the peak flow and the time to peak. Consequently, the following three rather simple criteria were selected for use in this study:

a)Runoff volumes - the ratio of volume observed and volume simulated
b)Runoff peaks - the ratio of peak observed and peak simulated
c)The time to peak - the ratio of the time-to-peak observed and time-to-peak simulated.

Runoff quality. The assessment of runoff quality simulations is even less developed than that of quantity simulations. From the runoff management point of view, the criteria can be defined for each constituent similarly as it was done for the quantity, i.e. describing the constituent pollutograph by the following three parameters:

a)The total constituent emission
b)The peak constituent concentration
c)The time to peak concentration.

These goodness of fit criteria for runoff quantity and quality were then used on the test catchments studied.

URBAN TEST CATCHMENTS

Description of Data Collection Projects

The Urban Drainage Subcommittee has obtained urban runoff data from a number of test catchments. These catchments and their basic characteristics are listed in Table 1.

Catchment name	Location	Sewer System
Bannatyne	Winnipeg, Man.	Combined
Brucewood	Toronto, Ont.	Separate
Calvin Park	Kingston, Ont.	Separate
East York	Toronto, Ont.	Separate
Halifax	Nova Scotia	Combined
Hamilton	Ontario	Combined
Malvern	Burlington, Ont.	Separate
Toronto-West	Ontario	Combined
Toronto-East	Ontario	Combined

Catchment name	Phenomena monitored			Area Size (acres)	Reference
	Precip.	Runoff	Quality		
Bannatyne	x[a]	x[a]	x[a]	542	14
Brucewood	x	x	x	48	14
Calvin Park	x	x		89	10
East York	x	x	x	40	16
Halifax	x	x		168	15
Hamilton	x[b]	x[b]	x[b]	176	3
Malvern	x	x	x	58	7
Toronto-West	x[a]	x[a]		2330	14
Toronto-East	x[b]	x[b]	x[b]	338	8

[a] limited number of events

[b] projects started recently, no data available as yet

Table 1.Urban Test Catchments.

The test catchments cover a wide range of catchment sizes (40 acres to 2300 acres) as well as of residential developments. Brucewood, Calvin Park and Malvern represent modern residential areas served by separate sewers. Bannatyne, Halifax, Toronto-West and Toronto-East are older residential areas served by combined sewers. East York is an older area on which the sewers were separated only recently. The storm sewers receive runoff mostly from roads and side-walks. The roof drains are connected to the old combined sewer.

On all the areas, precipitation and runoff were monitored. Quality data were collected with a various degree of success on all the areas except for Calvin Park and Toronto-West.

All of the projects are not at the same stage. The Brucewood and Bannatyne projects have been discontinued. The remaining data collection projects are continuing to a various extent although the data collected in East York have not yet been fully analyzed, and the Hamilton and Toronto-East projects which started only recently have as yet no significant data.

Some results from a previous study[10] with the SWMM model on two additional urban catchments (Oakdale, Chicago and Gray Haven, Baltimore) were also included. Thus for runoff quantity simulations, the data for the following eight areas were available for the testing of the SWMM model: Bannatyne, Brucewood, Calvin Park, Halifax, Malvern, Oakdale, Gray Haven and Toronto-West.

The runoff quality data are much less plentiful. In fact, only limited data and quality simulations were available for the Bannatyne, Brucewood and Malvern catchments.

Uncertainty in the collected data

A quantitative evaluation of uncertainties in the collected data was not possible due to the lack of information. Therefore, only a qualitative evaluation was made here, the uncertainty in the data was ranked and this ranking was then used in a later part of this study. The ranking of the data from the eight areas under consideration is shown in Table 2, where a low rank number indicates the better data set.

AREA	Rank
Bannatyne	7
Brucewood	5
Calvin Park	1-3 (assigned aver.rank=2)
Halifax	6
Gray Haven	1-3 (2)
Oakdale	4
Malvern	1-3 (2)
Toronto-West	8

Table 2.Ranking of data uncertainties for the studied urban areas.

The Calvin Park, Gray Haven and Malvern data were given the highest rank. In all these cases, the catchments were well defined and surveyed, the precipitation was measured on the catchment, and checked against another gauge, flows were measured by calibrated constriction flow meters, a good synchronization of precipitation and runoff records was evident. The measured data were checked for correctness.

The Oakdale and Brucewood data were rated slightly lower. It would appear that the flow meters were not calibrated and there is no evidence that the collected data were checked. It was expected that the data from the smaller Oakdale catchment were better defined (more accurate) than those from the Brucewood catchment.

The next data ranked are the Halifax data collected on an older area with some uncertainties in the catchment imperviousness. Otherwise, the instrumentation system is fairly good; a raingauge is located within the catchment and flows are measured by a critical flow meter.

The lowest rated data were those collected on the Bannatyne and Toronto-West catchments. There were no rain data collected directly on the Bannatyne catchment. Consequently, the data from some nearby rain gauges had to be used. In the case of Toronto-West, the flow rates were only inferred from the depth of flow measurements and the Manning equation. Only one raingauge was used to measure the precipitation.

DISCUSSION OF RESULTS

Runoff quantity

The results of runoff quantity simulations with the SWMM model are given in Table 3. For runoff volumes, peak flows, and times to peak, the ratios of observed to simulated values were computed. The results were described by the mean value of these ratios, standard deviation about mean and the percentage of simulations for which the simulated values were within ±20% of the observed ones (see Table 3).

	Runoff volumes		
	Ratio $Vol._{obs.}/Vol._{sim.}$		
	average	standard deviation	% of simulations within ± 20% of observations
Bannatyne	1.40	0.34	24%
Brucewood	0.91	0.19	66%
Calvin Park	1.03	0.17	75%
Gray Haven	—	--	--
Halifax	1.01	0.14	85%
Oakdale	--	--	--
Malvern	1.01	0.12	89%
Toronto-West	0.87	0.26	50%

	Runoff peak flows		
	Ratio $Qp_{obs.}/Qp_{sim.}$		
	average	standard deviation	% of simulations within ± 20% of observations
Bannatyne	1.12	0.09	81%
Brucewood	1.22	0.26	42%
Calvin Park	1.09	0.16	72%
Gray Haven	0.98	0.24	61%
Halifax	0.78	0.22	44%
Oakdale	1.04	0.19	70%
Malvern	1.05	0.16	77%
Toronto-West	1.12	0.14	70%

	Times to peak		
	Ratio $Tp_{obs.}/Tp_{sim}$		
	average	standard deviation	% of simulations within ± 20% of observations
Bannatyne	0.98	0.12	90%
Brucewood	0.91	0.10	87%
Calvin Park	0.93	.09	92%
Gray Haven	1.02	0.05	100%
Halifax	1.11	0.21	60%
Oakdale	0.92	0.13	81%
Malvern	0.96	0.07	99%
Toronto-West	1.13	0.22	55%

Table 3. SWMM runoff quantity simulations-goodness of fit.

For runoff volumes, the best goodness of fit was obtained for the Malvern catchment - nearly 90% of all the simulated volumes were within the ±20% limits. For peak flows, the best fit was found for the Bannatyne catchment, 81% of all simulations were within the above accuracy limits. Finally, for the times to peak, the best fit was found for the Gray Haven catchment, practically all the simulations were within the above accuracy limits. The overall goodness of fit was also evaluated. The Malvern catchment ranked the highest, the Toronto-West data ranked the lowest.

A large variation in the goodness of fit of the SWMM simulations on the test catchments led to a question of whether there is a correlation between the uncertainty in the input data and the goodness of fit. Since the data on hand did not allow the use of parametric statistics, this question was studied using non-parametric statistical methods. The null hypothesis was defined as follows: There is no correlation between the uncertainty in the input data and the goodness of fit of simulated to observed data. This would imply that the errors in the simulations are caused by a biased model structure.

The above null hypothesis was tested using the Spearman rank correlation coefficient. The calculation is given in Table 4.

Test catchment	Input data uncertainty rank	Goodness of fit rank (after Table 3)	Difference
Bannatyne	7	5	2
Brucewood	5	6	1
Calvin Park	2	3	1
Gray Haven	2	2	0
Halifax	6	7	1
Oakdale	4	4	0
Malvern	2	1	1
Toronto-West	8	8	0

$$\Sigma d_i^2 = 8$$

$$r_s = \frac{\Sigma x^2 + \Sigma y^2 - \Sigma d_i^2}{2\sqrt{\Sigma x^2 \Sigma y^2}} = \frac{73.0}{80.9} = 0.90$$

Table 4.Ranking of input data uncertainty and the goodness of fit.

For eight observations, the value of Spearman rank correlation coefficient of 0.90 is significant at the 0.01 level of confidence[12] and the null hypothesis has to be rejected. Thus there is a correlation between the uncertainty in the input data and the goodness of fit of the SWMM runoff quantity simulations. This indicates, that lower simulation accuracies obtained with the SWMM model on some areas, e.g. Toronto-West, are not necessarily caused by the modelling bias, but rather by inaccurate input data. A rigorous evaluation of the input data errors could not be done for any of the studied areas, since this would require much more extensive data records than those available (e.g. several precipitation records, etc.). Only on a thoroughly instrumented area one could directly separate the modelling bias errors from those caused by the input data errors.

One condition, under which the SWMM model fails, is the surcharged flow in sewers. A technique in which the sewer surcharging was avoided by arbitrarily increasing the sewer pipe capacity was used by Waller[15] in conjunction with the SWMM model on the Halifax catchment. As one would expect, it led to an overestimate of peak flows and a shortening of times to peak. These results, however, were more realistic than the truncated hydrographs produced by the normal SWMM runoff subroutine.

Runoff quality

Only limited runoff quality data have been collected on the studied areas so far and not all of these data have been processed to this date. In fact, quality data were available only for the following three catchments: Brucewood, Bannatyne, and Malvern. These data do not allow proper statistical analysis as was done for the quantity data. Consequently, only a qualitative discussion of the processed data follows.

The runoff quality data and the SWMM simulations are given in Table 5. The ratios of observed to simulated values were calculated for the total pollutant emissions and peak concentrations. For individual catchments, these ratios were characterized by the mean values.

	Bannatyne ISS=0	Bannatyne ISS=1	Brucewood ISS=0	Brucewood ISS=1	Malvern ISS=0
(a)					
Total BOD obs. / Total BOD sim.	3.10	5.25	.66	.29	--
Total SS obs. / Total SS sim.	1.34	2.20	6.43	.46	4.12
Total COD obs. / Total COD sim.					.49
Total N obs. / Total N sim.					4.80
Total P obs. / Total P sim					2.45
(b)					
Peak BOD obs. / Peak BOD sim.	2.90	6.43	1.58	1.35	--
Peak SS obs. / Peak SS sim.	1.05	--	9.60	.43	5.48
Peak COD obs. / Peak COD sim.					.28
Peak N obs. / Peak N sim.					3.82
Peak P obs. / Peak P sim.					3.01
Reference	14		14		7

Table 5.SWMM model runoff quality simulations described by mean values of the ratios (a) Total constituent emission observed to that simulated (b) The peak constituent concentration observed to that simulated.

The Brucewood and Malvern catchments are relatively clean areas, served by separate sewers. The observed Biochemical Oxygen Demands (BOD) for minor storms did not exceed 25mg/litre, the observed Suspended Solids (SS) concentrations did not exceed the value of 500 mg/litre. A large scatter in the observed and simulated data comparisons was evident. No conclusions can be drawn regarding the use of the options to calculate the suspended solids. The exponential decay option (code ISS=0) yielded simulated concentrations that were too high; the other option (an empirical relationship, code ISS=1) yielded simulated concentrations that were too low. On average, the calculated BOD concentrations were underestimated. The estimate of the suspended solids concentrations depended on the selection of the calculation option.

The concentration of Nitrogen and Phosphates were on average underestimated in the SWMM simulations. On the other hand, the Chemical Oxygen Demands (COD) were consistently overestimated in the simulations. It is expected that these runoff quality data will be further analyzed and attempts will be made to explain the lack of goodness of fit.

The Bannatyne catchment is served by combined sewers. Unusually high values of BOD and SS concentrations were observed on this area. As indicated in Table 5, the SWMM simulations underestimated the total BOD and SS emissions as well as the peak concentrations of both BOD and SS.

Uncertainties in the collected runoff quality data cannot be estimated and in fact, they could be fairly high. Consequently, one cannot conclude, if the errors are due to modelling bias or due to errors in the quality data. It may take another one or two years before a sufficient volume of runoff quality data is accumulated under the present program and a full evaluation of the SWMM quality subroutine is possible. Meantime, the runoff quality data obtained with the SWMM should be accepted and used only with great caution.

CONCLUSIONS

The runoff quantity subroutine of the Storm Water Management Model was tested with a good success on a number of new urban test catchments. The goodness of fit of the simulated to the observed data was found to be dependent on the uncertainty in the input data. No presently instrumented catchment allows separation of the errors due to the modelling bias from those due to the uncertainty in the input data. On the best instrumented catchment, fairly accurate results were obtained with the SWMM model. In fact, up to 90% of runoff volumes, 77% of runoff peak flows and 100% of times to peak were simulated with an accuracy better than ±20% of the observed values.

The SWMM model runoff quality simulations were found to be less satisfactory. Though the insufficient data prevent drawing any firm conclusions, it appears that the quality subroutine is not readily applicable to all urban catchments. The SWMM quality simulations should be treated with great caution, particularly if used for a selection of urban runoff control alternatives, or policy enforcement. It may require another one or two years of data collection before the SWMM quality subroutine can be fully evaluated for the feasibility of application on Canadian urban catchments.

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APPLICATION OF STORM AND SWMM FOR ASSESSMENT OF URBAN DRAINAGE ALTERNATIVES IN CANADA

Paul E. Wisner
Manager, Water Resources Group
James F. MacLaren Limited

Andrew F. Roake
Environmental Engineer
James F. MacLaren Limited

Adel F. Ashamalla
Senior Water Resources Engineer
James F. MacLaren Limited

Environmental Consultants, 435 McNicoll Avenue
Willowdale, Ontario, M2H 2R8

Abstract

A limited programme of research and several applications of urban runoff models indicate that there is no unique pattern for model application in drainage and pollution control studies. Use of the simplest model compatible with the requirements of planners and decision makers helps to minimize unnecessary data collection and avoid communication problems. More sophisticated models will be required as a study progresses from screening and initial planning phases to the final planning and design phases. STORM is considered as primarily a screening model for comparison of alternatives, identification of critical events and problem definition. For predominantly urban areas a lumped SWMM and a recently developed Generalized Quality Model are considered as planning models for the analysis of critical events. A detailed SWMM and the WREM are considered as tools for final planning and design work. A computerized unit hydrograph approach is preferred for planning in areas with low percentage imperviousness, while the comprehensive analysis of Stanford-type models is recognized as necessary for major projects in large watersheds.

Background

At present there is no specific urban runoff control legislation in Canada. A 1973 inquiry into urban drainage practice in Canada[1] revealed that at that time all major municipalities (with the exception of Toronto) employed the Rational Formula[2] exclusively in urban drainage planning and design. Within the last few years the Canada/Ontario Urban Drainage Programme has sponsored several studies related to the calibration/validation and development of urban runoff models [1,3,4] and the advantages of a modelling approach to drainage problems have been recognized by several large urban centres which have instigated programmes of model implementation. The principal models currently used in drainage studies in Canada are STORM[5], SWMM[6], WREM[7] and computerized unit hydrograph models.

The Water Resources Division of James F. MacLaren Limited has been extensively involved in the model development and verification studies for the Canada/Ontario Urban Drainage Programme and in a considerable number of practical model applications for cities and municipalities in Canada. It is the intent in this paper to present our views, as consultants on the relative priorities for model improvement and the implementation of modelling in drainage planning and design, and the role of some existing models in these fields.

Model Application and Improvement

Most urban runoff models encountered in the programmes of model testing[1,4] have required a significant effort in "de-bugging" before being rendered fully operational. Additional de-bugging is often required upon the release of later versions of an existing model. The correction of programme errors can be a lengthy and frustrating process and is apt to deter potential users and cause mistrust of models in planners and decision makers. Some operational models have proved to be well suited to certain applications but inaccurate in others. Table 1 summarizes the modifications and routines developed to enable existing models to be applied in Canadian conditions.

Table 1

Some Recent[4] Improvements to SWMM and STORM

1. Snowmelt Quantity and Quality model integrated with the SWMM RUNOFF block for Canadian conditions
2. Recommendations for lumping SWMM in simplied simulations
3. Modification of STORAGE and TREATMENT blocks reflecting new data
4. Modification of the TRCOST routine for Canadian Cost estimates
5. Development of a Data Analysis Model for processing of Canadian Atmospheric Environment Service data for direct input to STORM.

Models, such as STORM, are readily accepted by non-modellers because of their simple formulation and statistical interpretation of the model output. However, traditional hydrologists appear sceptical of these 'oversimplified' models. Because of the large investments involved in major watershed projects, the use of a much more sophisticated approach such as that offered by Stanford-type models[8] has been advocated. The dilemma appears to be that as more models are formulated, the chance of each of these being accepted by planners or decision makers at a municipal level becomes more remote. In the interim, outmoded empirical methods continue to be used for design purposes in some costly storm sewer projects and modelling is not used to its full extent in the examination of alternative solutions to such problems as sewer separation, and the need for upgraded treatment plants. We consider that at the present status of model implementation in Canada, further refinement of models and the construction of new models should be carefully weighed against the hidden constraints involved, i.e. additional de-bugging, time required for familiarization and potential reluctance to implement new and untested models. If currently applied models can be used in a creative and problem oriented manner and be demonstrated to be a means to novel design and economic benefits then at present these efforts will be more effective in promoting the widespread acceptance of modelling than further model refinement.

No Single Model

The designation of STORM as a "planning model" or SWMM as a "design model" may cause a user to be model oriented rather than problem oriented. Few models, if any, are completely universal and, therefore, some caution should be exercised when an existing model is applied in a new and untested role. The deficiencies of some well accepted models noted in Table 2 indicate some of the situations in which these models do not perform well. For instance, STORM does not simulate peak flows accurately because of its long time step (1 hour) and lack of flow routing routines. SWMM does not accurately simulate hydrographs under surcharged conditions. Conversely the highly sophisticated WREM is unsuitable for initial planning applications because of the extensive data preparation and considerable computer time required. While SWMM and WREM have been widely tested and verified on urban watersheds [9,10,4] little evidence of their suitability in predominantly rural situations has been published. Consequently we have used a computerized unit hydrograph approach in predicting rural runoff flows[11].

Table 2

Some General Model Deficiencies

Model	Comment
STORM	- peak flows not accurate due to 1 hour time step and no flow routing
	- simplistic storage and treatment routines
SWMM	- antecedent conditions have usually to be assumed
	- poor simulation of hydrographs in surcharged systems
	- not well validated for predominantly rural areas
	- quality model hard to calibrate, somewhat oversophisticated for most applications
	- receiving water model does not account for pollutant transport by diffusion
WREM	- very short time steps required to avoid unstability
	- extensive data requirements

Many models offer significant advantages if used sensibly within their proven limitations. Table 3 summarizes 12 practical modelling studies in which the authors participated. The model applications involved in these studies may be broadly categorized as; screening (1) - (3); planning (4) - (8); final planning/design (9) - (12). This work has emphasized the advantages of choosing the model most appropriate to the task in hand and of using several interfaced[12] models during a single study.

A Hierarchy of Models

The early planning stages of some urban drainage projects are typified by limited amounts of relevant data and several alternative patterns for development or solution of existing problems. The use of a simple model, such as STORM, at this stage represents an economic approach to screening alternative policies at a level of sophistication compatible with available data and acceptance by non-technical planners and decision makers. If the limitations of STORM are recognized it may also be used to screen long meteorological records for the identification of conditions antecedent to critical events. For instance, the relative importance of snowmelt compared with summer storm runoff may be assessed and important sequences of meteorological events identified. STORM can be used to determine the events to be simulated in more detail later in the project. This facilitates the selection of a historical "design" storm with known antecedent conditions, rather than the somewhat hypothetical synthetic design storm[13], for subsequent modelling with SWMM or WREM (see Figure 1).

Three recent studies conducted by James F. MacLaren incorporated this screening approach.

(1) Screening a Long-Term Meteorological Record

An assessment of frequency of flooding and problems associated with soil erosion during floods is being investigated for a watershed of about 9 square miles in Eastern Ontario. Urban encroachment onto the lower regions of the flood plain has aggravated flooding problems. The relative significance of spring snowmelt flows compared with the standard 1:25, 1:50 and 1:100 year design flows is required for the selection of the appropriate control measures. STORM was used to simulate all snowmelt events in a meteorological record of precipitation and temperature of 100 yrs. duration. Critical events can be extracted from the summary output and detailed event hydrographs computed. The model can then be used for initial estimates of the effects of storage reservoirs on critical flows.

(2) Screening a Number of Development Alternatives

Twelve alternative development concepts were proposed in the initial planning stage for the new North Pickering Townsite, east of Toronto. STORM was used to provide an initial assessment of the probable annual changes in urban runoff volume and quality associated with each of the alternatives in the three main watersheds affected (West Duffin Creek - 58 square miles, East Duffin Creek - 46 square miles, Petticoat Creek - 10 square miles). The proposed land uses were supplied as input to the model for each case and the annual pollutant load (B.O.D., S.S., Settleable Solids, N, PO_4) and the total annual runoff was computed. Similar computations were performed for the existing land use pattern, which provided a base case. A simple ranking model was developed to facilitate comparison and ranking of the development alternatives on the basis of their overall water quality impact. It was demonstrated, using STORM, that for any alternative, a storage-treatment relationship (i.e. a set of storage-treatment combinations) exists for which the overall water quality impact of that alternative can usually be reduced to a predetermined level (existing condition or a pre-defined 'allowable loading'). The effect of low frequency floods was investigated in the same study. The unit hydrograph method is generally applied for flood synthesis in Ontario. A computerized version of this method (FROUT) was developed to predict the effects of low frequency floods and associated erosion before and after urbanization. The results of this study formed part of an overall planning matrix involving considerations other than water quality impacts of urbanization, with a view to selecting the preferred alternative.

(3) Identification of Critical Areas

Sewer system inadequacies and changing land use patterns often result in a considerably higher number of combined sewer overflows from some areas in a city than from other areas in the same city. The most cost-effective approach to limiting the pollution of receiving waters due to combined sewer overflows is to limit overflows from the critical areas. The first stage in such an effort is obviously to define the critical areas. STORM was used for this purpose for the City of Winnipeg. Five years meteorological records were processed for the simulation of the quality of runoff and snowmelt in 35 combined sewer areas. Calibrations to City records enabled period total emissions of B.O.D. and SS to be reproduced to within ± 10 percent of the measured totals. A number of critical areas were identified on the basis of average annual pollutant discharge and mass discharge per overflow event and critical events were subsequently simulated in more detail with SWMM in order to evaluate various control alternatives.

It has been shown that fairly sophisticated single event models, such as SWMM, can be applied in a lumped[5,14] manner (i.e. the input characteristics describing the subcatchments and transport system can be aggregated) for simplified simulation. This implies that in situations where only basin outlet hydrographs from design events are required, such as in the initial planning stages, data preparation time may be minimized. At this stage, it is considered that the sophisticated pollutant routing routines of SWMM are not justified. Consequently, the use of a Generalized Quality model (Appendix 1) in conjunction with lumped SWMM, or unitgraph models is advocated.

In the final planning stages of the project, more detailed information and monitoring results become available and the number of alternatives is reduced. At this stage a detailed simulation involving fine discretization and calibration for accurate water quality prediction is warranted. At this juncture, the effects of untreated and treated discharges to the receiving water would be assessed. A more sophisticated one-dimensional or two-dimensional receiving water model than that in SWMM (i.e. RECEIV) might be required in some cases[15].

The WREM model is sometimes employed in final planning for an analysis of the benefits of surcharged design. According to our experience in studies conducted in Winnipeg, Port Credit and Edmonton, the intentional use of surcharge in the design of relief sewers[16,17] or in the analysis of interceptor capacity[18] can lead to considerable reduction in peak stormwater flows. Consequently, it appears reasonable to employ only a model with sophisticated routing, such as the WREM, capable of simulating surcharged flow in the design of relief sewers or in the final planning phase of new projects where in-line storage by surcharge is feasible.

During the course of a project from screening to design, model sophistication, data requirements and computer costs will all increase. The results of each model should lead logically to the next, more sophisticated application and good communications with the decision makers should ensure a shared objective. The involvement of non-technical planners and decision makers in regular consultations is essential in this regard.

Our experience in studies for the City of Winnipeg indicates that once flow simulation techniques are understood and the potential benefits appreciated, there is a natural tendency of planners and decision makers to become interested in quality simulation as a part of pollution control policy planning.

Conclusions

One of the primary goals of those involved in urban runoff modelling in Canada should be the replacement of outmoded empirical design formulae currently widely used in Canadian urban drainage planning and design by more accurate and reliable methodologies. At present this goal will be best served by the implementation in engineering practice of existing well validated models. The experience in a number of research and practical urban drainage and pollution control studies confirms that modelling is a dynamic process. No single model or unique pattern of application can be recommended. Best results are likely to be achieved with a series of interfaced models applied within proven limitations. This approach may logically result in the ultimate acceptance of highly sophisticated continuous simulation models in the final planning phase of most major watershed studies.

Table 3

Examples of Practical Model Application and Interface

STUDY	SCOPE	MODELS	SIMULATIONS
(1) Effects of urbanization. Screening development alternatives for North Pickering Community (Phase 1)	Comparison of low frequency floods & water quality impacts of 12 development alternatives	FROUT	1:10, 1:25, 1:50 years floods and associated solids erosions
		STORM	Modification of total annual runoff & runoff pollutant loads & effects of storage & treatment (1 year)
(2) Comparison of Flood Control Alternatives on the partially urbanized Graham Creek watershed	Relative magnitude of snowmelt runoff compared to summer storm runoff	STORM	Screening of 100 yrs meteorological data
		SWMM (snowmelt)	snowmelt, urban areas
		FROUT	non-urban area runoff, flow routing
(3) Evaluation of combined overflow pollution in Winnipeg	Problem identification. Critical areas and major events. Preliminary analysis of control alternatives	STORM	Comparison of annual pollutant loads in overflow over 5 years in 34 districts
		SWMM	Simulation of critical events for different control policies
		RECEIV	
(4) Master Drainage Plan for Thornhill-Vaughan development, Ontario	Effects of development on peak flows. Outline for main drainage lines and storage facilities	FROUT	1:25, 1:100 year floods
		SWMM (lumped)	Sizing of main trunk storm sewers and runoff detention ponds
(5) P.A.C.E. Study of Runoff from Oil Distribution Terminals	Simulation of overflows Quantity and Quality of Terminal Runoff	STORM	Simulation of annual overflows-reduced time step employed for small areas
		SWMM	Runoff hydrographs
		GQM	peak concentrations and event total pollutant load

Table 3 (cont'd)

STUDY	SCOPE	MODELS	SIMULATIONS
(6) Toronto International Airport Runoff Study	Demonstration of relationships between airport operations and runoff pollution. Comparison of control alternatives	STORM SWMM GQM	Snowmelt events Storm runoff simulation Event total pollutant loads
(7) Humber River Outfall, Toronto	Planning study for the optimum location of nearshore landfill developments	RECEIV	Simulation of critical water quality conditions for different landfill configurations
(8) Winnipeg Drainage Criteria Manual	Development of drainage policies and procedures involving small ponds and roof storage	SWMM	Examples of sewer and storage design methodologies (<200 acres)
(9) Port Credit Storm Relief Study	Analysis of existing storm sewer system. Requirements for upgrading system performance	SWMM WREM	Runoff and non-surcharged flows Analysis of surcharged conditions, testing of relief alternatives
(10) Relief Sewers in Jessie, Winnipeg	Analysis of existing combined system in Jessie district. Design of relief lines	SWMM WREM	Runoff and non-surcharged flows Analysis of surcharged conditions, design with surcharge
(11) Edmonton Interceptor Study	Analysis of existing system & relief requirements. Investigation of regulators and overflows	SWMM WREM	Inlet hydrograph from detailed areas Analysis of surcharge and overflows during design and historical storms
(12) Winnipeg Stormwater Pumping Station Study	Analysis of pumping station performance and effect of inline storage	WREN	Simulation of flows during critical historical storms, surcharged conditions.

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Appendix 1

Generalized Quality Model (GQM)

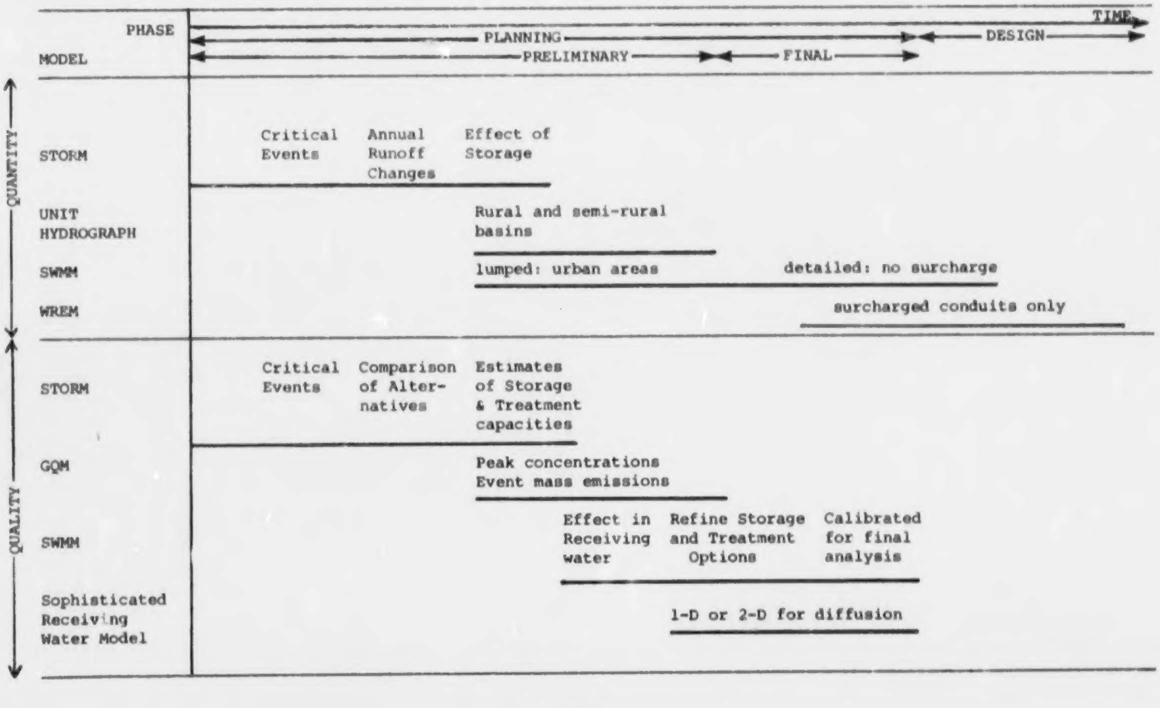
The Generalized Quality Model computes surface runoff quality in basically the same manner as the SWMM. Some of the important aspects of the new model are summarized below:

(a) Aggregated single catchment model
(b) Five land uses possible
(c) Separate input hydrograph forms basis for quality computations. (This may be generated by any model or originate from measurements. Any time interval can be used for hydrograph input)
(d) User supplied dust and dirt composition and loading rates for each land use
(e) No quality routing or pollutant decay computations
(f) No erosion or deposition of sediments computed
(g) Two methods for Suspended Solids computation
(h) Catchbasin contributions modelled
(i) Quality calculations may be based on either flow from the total area, or only on flow from the impervious area
(j) Ten pollutants may be simulated (BOD, COD, Suspended Solids, Settleable Solids, Coliforms, N, PO_4, Cl, lead, oil and grease)
(k) No default values supplied
(l) Pollutographs, mass curves and surface load statistics are available for each pollutant

The principal advantage of the Generalized Quality Model is the reduced cost of computations and reduced data preparation time achieved by aggregating the properties of the entire study area and modelling it as a single catchment. The model is extremely flexible and may be used for the study of many aspects of stormwater pollution.

FIGURE 1

THE ROLE OF MODELS IN DIFFERENT PHASES OF DRAINAGE STUDIES


TIME
PHASE
PLANNING
DESIGN
MODEL
PRELIMINARY
FINAL
QUANTITY
STORM
Critical Events
Annual Runoff Changes
Effect of Storage
UNIT HYDROGRAPH
Rural and semi-rural basins
SWMM
lumped: urban areas
detailed: no surcharge
WREM
surcharged conduits only
QUALITY
STORM
Critical Events
Comparison of Alternatives
Estimates of Storage & Treatment capacities
GQM
Peak concentrations
Event mass emissions
SWMM
Effect in Receiving water
Refine Storage and Treatment Options
Calibrated for final analysis
Sophisticated Receiving Water Model
1-D or 2-D for diffusion

ON THE VERIFICATION OF A THREE-DIMENSIONAL PHYTOPLANKTON MODEL OF LAKE ONTARIO

Robert V. Thomann
Environmental Engineering & Science Program
Manhattan College
Bronx, N.Y. 10471

Richard P. Winfield
Environmental Engineering & Science Program
Manhattan College
Bronx, N.Y. 10471

INTRODUCTION

The purpose of this paper is to highlight the growing need for detailed and quantitative verification of water quality models that goes well beyond model computation and determines measures of model adequacy for the decision maker. In particular, this paper is focused on the need for verification of phytoplankton-nutrient models, the number of which has increased significantly in recent years. These models all make use of a similar underlying deterministic framework of coupled interactive non-linear differential equations which are solved numerically in discrete space and time.

Indeed, the state of the computing art of such frameworks is advancing rapidly and today it is no longer of great moment if hundreds of sets of non-linear equations are successfully solved on a large computer. What is of significance however, is whether the numerical computations are "reasonable" representations of the real world. It is at this point that considerable confusion results both in the realm of the model builder and in the mind of the decision maker. What is "reasonable"? Is it sufficient to generate computed values that "look" like what we are observing? For example, is it sufficient that a phytoplankton model simply generate a spring pulse which has been observed or is there a certain quantitative measure that must be introduced to determine not only that a spring pulse is calculated but that it's magnitude is correct in some sense? The question addressed in this paper therefore is "What criteria might one use to determine the adequacy of the model?" It is strongly believed that unless a detailed examination of the comparison of the model to observed data is carried out, there is no way of judging the adequacy of the computation. There may, of course, be situations where this is not possible; as for example in projecting phytoplankton conditions in a reservoir that is not yet in existence. Such a problem context is not considered here. The thrust of this paper is aimed at detailed verification, where possible, so that the credibility and utility of a modeling framework are established.

THE LAKE ONTARIO MODEL

A three dimensional model of the phytoplankton of Lake Ontario is used as an illustration of the kind of problem that one faces in attempting a detailed verification analysis. The basis of this model, called Lake 3 has been discussed previously(1). The kinetics of the model include linear and non-linear interactions between 1) phytoplankton chlorophyll, 2) herbivorous zooplankton, 3) carnivorous zooplankton, 4) detrital nitrogen, 5) ammonia nitrogen, 6) nitrate nitrogen, 7) detrital phosphorus and 8) orthophosphate phosphorus. The details of the kinetics are given in (1) where a lakewide model (using only vertical definition) was used to verify, by judgment, open lake behavior.

Fig. 1 shows the spatial configuration of the computational grid used for Lake 3; 67 segments are used and for the eight dependent variables, 536 non-linear equations are integrated in time for a maximum period of 14 months.

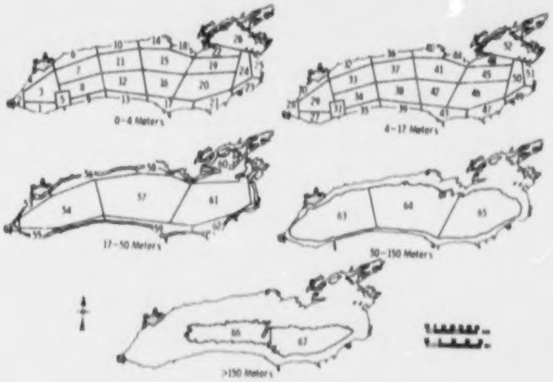


Fig. 1 Lake 3 Model Grid

A time step of .08 days is used throughout and solution is accomplished on a CDC 6600 and requires some 63K of storage and about 1 hour of equivalent main frame computing time. The model is relatively large and for any one run generates some 100,000 numbers. The analyst attempting to absorb the behavior of such a model faces a formidable, indeed almost impossible task since attention can only be directed towards certain portions of the model (either in variable or physical space). Furthermore, since the various portions of the model are so interactive, "adjustments" to improve the model in one region may result in an undersirable change in another of the model. Therefore, a strategy for determining the behavior of the model and its verification status must be developed. Such a strategy must of necessity include the utilization of an available data base such as the results from the International Field Year on the Great Lakes (IFYGL) for Lake Ontario. Fig. 2 shows the flow diagram adopted for the analysis of the Lake 3 model.

REDUCTION OF IFYGL DATA BASE

The IFYGL data base is resident in STORET and contains approximately 200,000 observations, encompassing 75 water quality parameters. This data base is the most complete set of observations obtained to date on Lake Ontario and contains a wealth of information on the

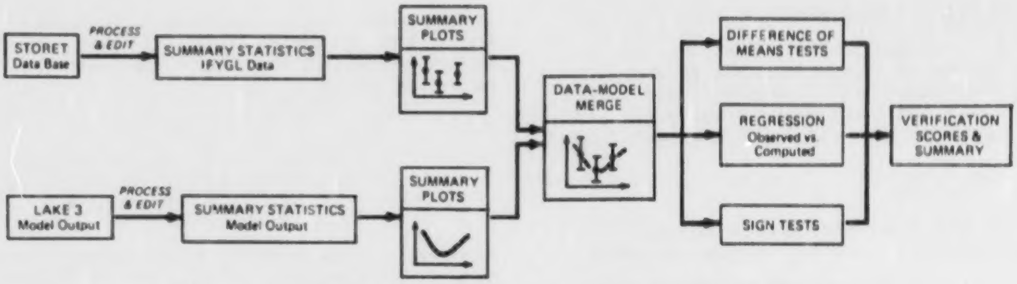


Fig. 2. Flow diagram for model verification analysis

dynamics of the Lake. The task as shown in Fig. 2 is to utilize the data set to produce summary statistics of the IFYGL data, which would be used to analyze the results of the Lake 3 model. These statistics are generated for volumes of the Lake corresponding to the segmentation of the Lake 3 model. Given the IFYGL cruises, monthly mean and variance statistics are used. After the segment statistics are generated for the various water quality parameters of interest, a display package is accessed to generate microfilm or paper plots of the parameter statistics versus time.

The STORET data base is accessible to the user, through program packages for standard retrievals and manipulations of the data with fixed output format. Since the data set is large (2×10^5 observations) a methodology had to be formulated that would facilitate the sizable reduction task. Recognizing that the reduced statistical data set would be used on an entirely different computer system (CDC 6600) than EPA's 370-155 and the need to accomplish the data reduction in the shortest time possible,such a methodology is a necessity.

The scheme was carried out for each of the 67 segments and a total of over 200 runs were made. Each segment required three reduction runs since a maximum of eight parameters per run could be made and twenty variables were reduced per segment.

The first step was to prepare decks which described the segment volumes. Each volume was defined using a latitude/longitude polygon with depth constraints. The STORET program Mean was used to generate the segment statistics; monthly mean, standard deviation, number of observations, maximum and minimum. Since the output from Mean is fixed and the results were to be transported to the CDC-6600 via data cards, manipulation of the output file was necessitated. OSI's 370-155 operating system contains an online interactive text editor named Wylbur. Using Wylbur and its limited macro capability, text editing module programs were developed that reduced the output from 140 to 80 characters per line and eliminated all extraneous lines of information. This compressed data set was then punched and therefore, was in a form processable by the CDC-6600. A Fortran program was written to manipulate this data into the format required by the verification analysis and graphic display programs. The result of this effort was an IFYGL data set of monthly statistics for twenty variables for 67 segments for the period May, 1972 through June, 1973.

A graphical display program was also written in Fortran to display the temporal variation of the parameters. Monthly means plus or minus one standard deviation are displayed. The graphical output of this program can be routed either to paper or microfilm. The use of microfilm for both graphical and printed output has proven to be of immense utility when dealing with large scale problem such as Lake Ontario and is to be recommended.

VERIFICATION ANALYSIS

In the lower path of Fig. 2, the continuous Lake 3 model output is also processed to generate monthly mean values by segment, month and variable. A merge of data and model output is then accomplished, computer generated plots of theory and data are prepared for the analyst and a verification program is then accessed for testing the behavior of the model and for preparation of verification scores and summaries. Fig. 3 shows a typical plot(redrawn)as generated from one of the runs for segment #21 and shows the overplot of the theory and the observed data. The amount of effort to reach the stage of Fig. 3 is significant and should not be underestimated.

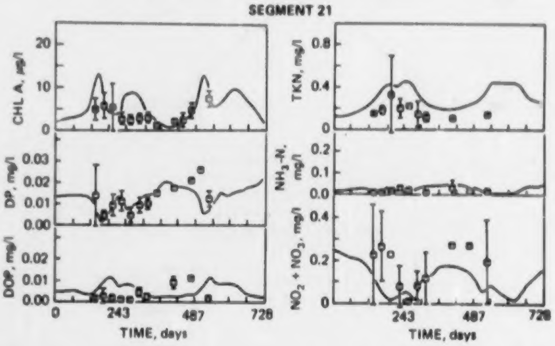


Fig. 3. Typical merge of model output(solid line) and data

Several simple tests comparing model output to observed data have been constructed and in this paper, emphasis is placed on testing the difference of means. A standard "t" test is used. Thus, let $\bar{x}_{ijk}$=observed mean for variable i, segment j and month k and $\bar{c}_{ijk}$=the comparable computed mean. Then $\bar{d}=\bar{c}-\bar{x}$ is the difference of means assumed to be distributed as a Student's "t" probability density function. If the variance of the model is assumed equal to the observed variance, then,

$$t = \frac{\bar{d} - \delta}{s_{\bar{d}}} \tag{1}$$

where δ is the true difference between the model and the data and $s_{\bar{d}}$ is the standard deviation of the difference given by the pooled variance or

$$s_{\bar{d}} = \frac{2s_x^2}{N} \tag{2}$$

for s_x^2 as the data variance for specific month, segment and variable. Under the null hypothesis: $\delta=0$, there is a "critical" $\bar{d}$ which delineates the region of rejection of the hypothesis and is given by

$$\bar{d}_c = \pm t\, s_{\bar{d}} \tag{3}$$

and for a 95% confidence range (5% chance of making a Type I error),

$$\bar{d}_c = \pm 2\, s_{\bar{d}} = \frac{2.83}{\sqrt{N}}\, s_x \tag{4}$$

The distribution of $\bar{d}$ and the critical regions are shown in Fig. 4. As indicated if $(-\bar{d}_c < \bar{d} < \bar{d}_c)_{ijk}$ the model is considered verified for variable i, segment j and month k and a score of V=0 is given. A positive value of V therefore indicates an overestimate of the mean while a negative value of V indicates an underestimate of the mean. The V score is therefore a measure of the degree to which the model deviates from the observed data given the temporal and spatial variability within a month and segment. More precisely, V is the extent to which the analysis has penetrated into the region of rejection of the null hypothesis. Of course, all the caveats of the application of such statistics apply, especially the chance (unknown) of making a Type II error (that the null hypothesis is not rejected when it should be). The V score is given by

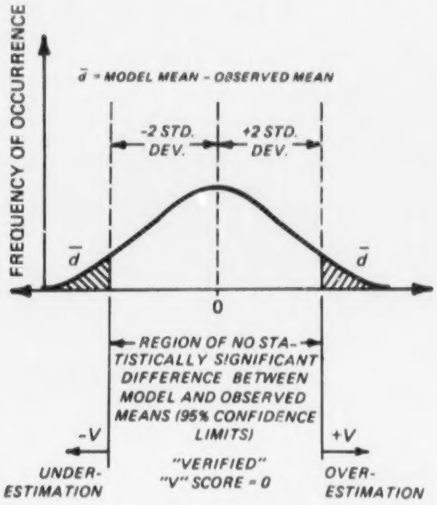

FREQUENCY OF OCCURRENCE
$\bar{d}$ = MODEL MEAN - OBSERVED MEAN
-2 STD. DEV.
+2 STD. DEV.
$\bar{d}$
$\bar{d}$
0
REGION OF NO STATISTICALLY SIGNIFICANT DIFFERENCE BETWEEN MODEL AND OBSERVED MEANS (95% CONFIDENCE LIMITS)
-V
+V
UNDER-ESTIMATION
"VERIFIED" "V" SCORE = 0
OVER-ESTIMATION

Fig. 4. Determination of verification score V

$$V_{ijk} = 0 \text{ for } |\bar{d}_{ijk}| < \bar{d}_c \tag{5}$$

$$V_{ijk} = \bar{d}_{ijk} - \bar{d}_c \text{ for } \bar{d} > \bar{d}_c \tag{6}$$

$$= -\bar{d}_{ijk} + \bar{d}_c \text{ for } -\bar{d} > -\bar{d}_c \tag{7}$$

Another simple measure that may be used is the number of segments in a given month that have a V score equal to zero. Therefore, let

$$K_{ijk} = 1 \text{ for } V_{ijk} = 0.$$

A score defined as the S score for variable i and month k is therefore given by

$$S_{ik} = \sum_{j=1}^{n} K_{ijk}/n \tag{8}$$

where n is the total number of segments where a V score can be computed, either for the entire lake or for just certain vertical layers or regions of the lake (as for example, near shore vs. open lake). The score then simply represents the fraction (or percent) of segments that "passed" the verification test of V=0. Since up to perhaps 10 variables are analyzed in this verification analysis, an overall aggregated S score can be also computed. Verification of all variables may not be of equal concern. For example, one may be willing to accept a lack of verification of ammonia nitrogen for the Lake but may be particularly concerned about say, total phosphorus and chlorophyll. Therefore, a series of weights, w_i, can be assigned to each variable i representing the relative importance of each variable. The aggregated score for month k is then given by

$$S_k = \sum_{i}^{r} \sum_{j}^{n} w_i K_{ijk}/(n\sum w_i) \tag{9}$$

where r is the number of variables that are in the aggregated score. S_k therefore represents the weighted fraction of the total number of segment variables that passed a "t" test of V=0 for month k. It should be noted that not all segments and variables can be tested at each month, so that r and n are functions of the data availability for month k.

RESULTS FROM LAKE 3 MODEL RUNS

For this paper, three runs of the Lake 3 model were available for verification analysis with the IFYGL data. These runs emphasized the sensitivity of the verification to the initial conditions for each variable and segment. For all runs, the average temperature variation, solar radiation, flow transport and horizontal and vertical dispersion were used(1). This is in contrast to using the actual conditions during the 1972-1973 IFYGL year. The kinetic structure used for the homogeneous Lake 1 model was also employed. The runs are: 1) Run #1, which used initial conditions equal throughout the Lake for January 1, such conditions being chosen from Lake 1 runs, 2) Run #2, which incorporates some spatial changes in initial conditions for chlorophyll, orthophosphate and nitrate based on IFYGL data, computation also begins on January 1; 3) Run

#3, which begins computation on May 1, 1972 and uses as initial conditions the observed segment averages for May, 1972 as given by the IFYGL data. Run #3 presumably then represents a "better" run in the sense that the initial conditions are chosen from the observed data. Not all segments had equal amounts of data and in some cases, significant data gaps existed for various months. Fig. 5 shows some typical results of the verification analysis for phytoplankton for segment #16; Run #1. The gaps in the record can be seen as well as the region of no statistically significant difference between model and observed mean (Eq.(4)) and the monthly differences between the model mean and the observed mean. "Insufficient data" indicates that the variance of the sample mean could not be computed, implying that only one sample was available. The range of the no difference region is significant and as shown can be as much as ± 4μg chlor/l. The application of Eqs. (5) to (7) would therefore lead to V scores of zero for months such as July to a maximum overestimation of 3.7 μg/l in June.

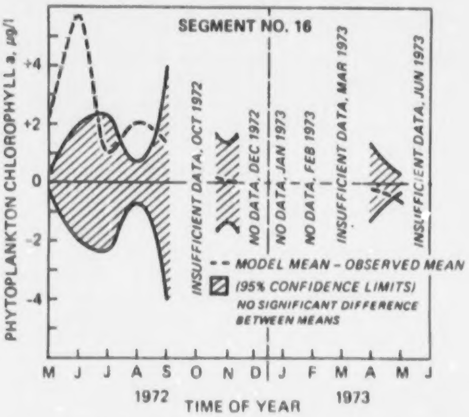


Fig. 5. Typical statistical comparison of model and data, Run #1

Computations such as represented in Fig.6 are carried out for each segment so that the analyst can also view the V score spatially by month. A typical result for Run #2 and June 1972 conditions is shown in Fig. 6.

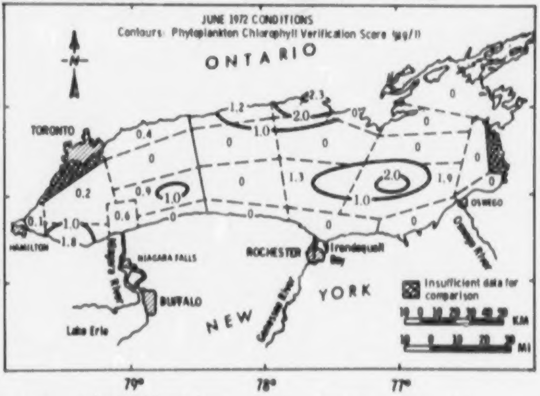


Fig. 6. Distribution of V score, Run #1,

As shown, a significant region of the Lake is verified for this run although there are certain sectors where the model overestimated the mean.

In order to provide further insight into the behavior of the model compared to the observed data, lake wide averages of each of the segment statistics were computed for two layers. Figs. 7 and 8 show some of these results for phytoplankton and Run #1.

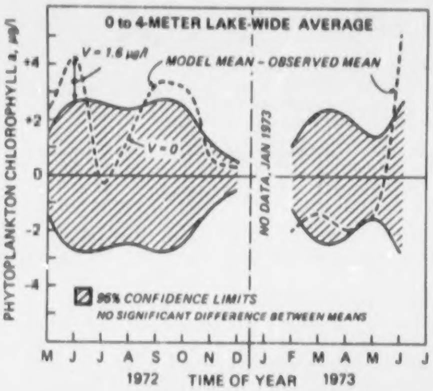


Fig. 7. 0-4 meters, lake wide comparison of model and data, Run #1

The lake wide average for the 0-4 meter depth layer shown in Fig. 7 shows that for the lake as a whole the region of no statistical difference is about 2μg/l and that for Run #1, the spring and fall bloom is generally overestimated by the model. Note also that the computation for the 1973 year just barely stayed within the region of no difference until June, 1973 where the model overestimated the mean by over 2μg/l. The rapid change from May, 1973 to June, 1973 indicates that, in general, the model was somewhat out of phase with the observed data during the period.

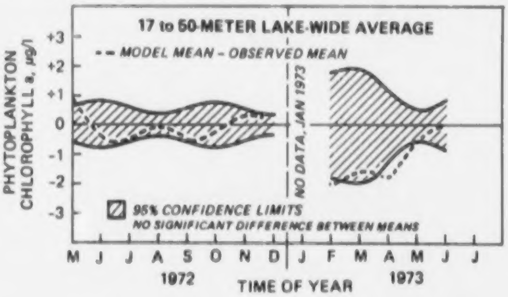


Fig. 8. 17-50 meters, lake wide comparison Run #1, Phytoplankton Chlorophyll

Fig. 8 shows a similar plot for the 17-50 meter depth; the relatively narrow band of no difference can be noted as well as the fact that the model did verify in all months except for some relatively slight deviations in 1973 and May, 1972 all of which were less than 1μg/l.

Fig. 9 shows the results of the V score for phytoplankton where the lake wide average is across each of the segment V scores for each month as opposed to Fig. 7 and 8 where the average was first taken of all of the means and a single score computed. All three runs of the model are indicated. Several key points can be seen: a) the adjustment of initial conditions from Run #1-#3 did not substantially improve the verification except in a few months, b) the fall phytoplankton bloom is consistently overestimated, while c) the spring 1973 conditions are somewhat underestimated and d) for most of the 14 month run, the model averaged about 1μg/l chlorophyll outside the limits of the region of no difference between model and observed means. A final illustration of the overall verification results is given by the S score of Eq. 9 as shown in Fig. 10. This S score represents the percent of the total number of segment-variables that had individual V scores of zero. During the 1972 period of verification approximately 50% of the segment-variables verified while during the 1973 period only 30-40% verified. (It should be noted however, that the data available in 1973 is significantly less than that in 1972.) Further, Run #3 which was constructed to further improve model performance did not really improve the overall verification; in fact it decreased the S score. None of the runs provided a substantial change in the S score. The S score therefore, represents a measure that incorporates the behavior of each of the key variables and provides a basis for determining whether the model verification is improving or deteriorating under different model input. It does not however indicate quantitatively the degree to which each segment variable failed to verify. The quantitative V score provides such an estimate. Plots such as Figs. 9 and 10 therefore complement each other in terms of displaying the overall verification of the model.

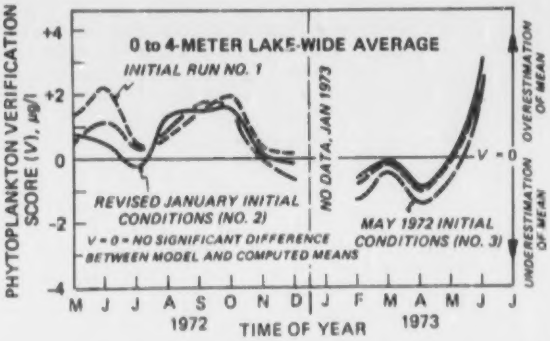


Fig. 9. Comparison of V scores for Runs #1-#3, 0-4 meters, Phytoplankton Chlorophyll

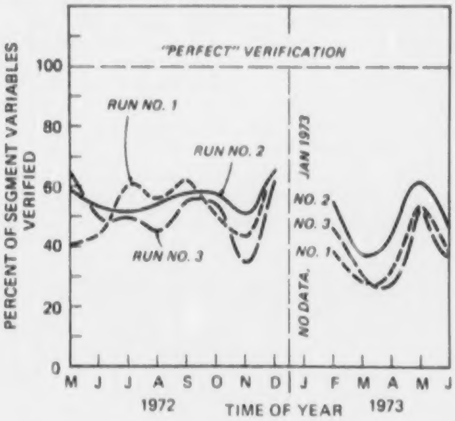


Fig. 10. Overall segment-variable score for Runs #1-#3

CONCLUSIONS

This paper has not addressed directly the question of whether the present Lake 3 model of Lake Ontario is a "good" model, but has rather concentrated on highlighting the need for development of measures of model verification. The analysis of the verification statistics of Lake Ontario does provide however an illustration of this very important need. It is no longer sufficient to simply develop numerical solutions to the complex interactive equations of phytoplankton models. Rather, a substantial effort must be expended to utilize available data bases together with statistical measures of verification in order to determine the overall credibility and adequacy of the model. The illustrative results presented here for Lake Ontario indicate how these measures of verification performance behave under different assumptions on model initial conditions. Overall, phytoplankton chlorophyll was verified to about 1μg/l chlorophyll outside of the limit of no difference between model mean and observed mean and approximately 40-50% of the segment-variables were verified regardless of the initial conditions.

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ACKNOWLEDGEMENTS

The assistance of William Beach, Jan-Tai Kuo and John Segna of Manhattan College is acknowledged together with the insights of our colleagues Drs. Donald O'Connor and Dominic Di Toro. This work was carried out under EPA Research Grant No. R803680-01.

MATHEMATICAL MODEL FOR THE EXCRETION OF $^{14}CO_2$ DURING RADIO RESPIROMETRIC STUDIES

Rumult Iltis
U. S. Environmental Protection Agency
Health Effects Research Laboratory
Cincinnati, Ohio

ABSTRACT

"Mathematical model" described in this paper applies to a biological process that can be expressed in a well defined analytical form. Specifically, it pertains to the rate of excretion of 14_C (injected i.v.) from the lungs of rats during the radiorespirometric investigations. In the experiment, the rate of excretion of $^{14}CO_2$ from the lungs is changed by a toxic agent (methyl mercury) ingested 24 hours prior to the experiment. In this study, the model for $^{14}CO_2$ excretion is presented in the form of a solution to four first order differential equations reduced to a fourth order differential equation. The integral of the model for the controls and the exposed animals at a selected time t_1 is used to measure the severity of toxicity by taking the difference of the two integrals. The model has 8 constants, thus it is possible to take 8 independent measurements, at the early stages of the experiment, and obtain eight independent equations to yield a solution (i.e. the distribution of the excretion with time). In this way a prediction of the effect, if any, can be made. Using heuristic approach, however, the model can be simplified to yield a skewed distribution that can be fitted to data up to the selected time t_1. The heuristic distribution contains only two parameters (unknowns), thus only two measurements at the beginning of the study are sufficient to predict the effects at any other point in time.

INTRODUCTION

Biological investigations including radiorespirometry require collection of large amounts of data in order to arrive at a statistically significant conclusion. This statement implies that experiments must be lengthy with large number of animals - a costly exercise that is not always possible. Mathematical modeling serves to circumvent this difficulty by predicting effects based upon small sets of data. As to its validity in an "absolute sense" it can be only stated that as long as it represents a simplification of reality its "utility" - i.e. the extent to which it helps the user - is the only fruitful criterion on which it can be judged. The modeling of radiorespirometry provides a convenient and economic method of screening large number of toxicants by reducing the time required for each experiment and the number of experiments required to make proper assessment.

In the experiment proper, investigators have been able to successfully explain the effects of metabolic conversion of ^{14}C-labeled substrates to respiratory $^{14}CO_2$ and the influence of various factors on the metabolism (Wang, 1967; Dost et al., 1973). The development of this method contributed significantly towards being able to observe chemical reactions that take place in experimental subjects without sacrificing the subjects. An animal can be used for both control and experimental purposes and, furthermore, the cumulative effect of repeated administration of an agent or recovery from a certain effect can be observed.

Materials and Methods

Forty-eight male rats (Charles River Laboratory) were used in this series of experiments. The radiolabeled substrate (^{14}C-1-glucose) used in this study was obtained from New England Nuclear Corporation.

The theoretical consideration, design of experiments, detailed methodology, and other background information have been published by this laboratory (Lee et al., 1972) and others (Wang, 1967; Tolbert et al., 1956).

Exhaled $^{14}CO_2$ was monitored continuously using Cary vibrating reed electrometers in conjunction with ionization chambers. The analog output of the electrometers was fed into a data acquisition system that printed the data in digital form on paper tape which was then decoded on a PDP8I computer. The block diagram of the flow system and the instrumentation are shown in Figure 1. The decoded data was later used for modeling and curve fitting on an analog and digital computer. The derivation of the model is based on biological processes in the course of excretion of $^{14}CO_2$ from the lungs of experimental animals. In the experiment, ^{14}C is introduced into the animal by i.v. injection. The rate of $^{14}CO_2$ excretion from the lungs is then modified by a toxic agent (methyl mercury in this case) via ingestion, 24 hours prior to i.v. injection of ^{14}C.

In the model it is assumed that there exists a "two-pool open system" (Shipley et al., 1972) in which one pool is the central compartment (blood pool) and the other is the conglomerate of all peripheral pools; liver, kidney, lung, etc. Any communication between peripheral pools occurs only through the central compartment as shown in Fig. 2. On solving the problem a system of 4 first-order differential equations is obtained leading to a solution for a skewed distribution that has eight constant coefficients as unknown. To predict the excretion rate and the severity of toxicity at a later time, eight measurements of excreted rate data at the beginning of the study are made. Eight independent equations are set, yielding the eight constant coefficients. The distribution (hence the solution) for any desired time is then obtained. The integrals of the distribution at a selected time t for the control and the exposed animals are compared. The difference, if any, represents the severity of the effect.

The validity of the model is proven by testing it on an analog computer and fitting data from four experiments to the model on a digital computer.

Another advantage of the method is the possibility of predicting effects for a given concentration of administered toxic agent, provided the controls and some intermediate curves for a particular animal are available. At this point it can be stated that the model is valid for any agent and for any animal that has the process behaving the way it is presented in this paper. Only the rate coefficients could be different for different animals or agents.

A clinical compartment follows linear kinetics in which the rate of flow from a compartment is proportional to the partial pressure of an agent (CO_2 in this case) within the compartment (Piotrkowski, 1971, Atkins, 1969). The output from each compartment is a solution to the first order differential equation of the form:

$$\frac{dy}{dt} = f(t,y) \text{ ------------------------------ } (1)$$

where y is the output or the amount of an agent excreted as a percent of total pollutant and t is the running time.

The lung is not a single compartment (Riley, R. L, 1920), but is composed of three classical ones. The first one consists of the alveoli -- the gas exchange compartment [blood releases and takes in gases via the capillaries surrounding the alveoli]. The second one is the anatomical "dead space" in the alveoli. The third one is the "dead space" in the respiratory tracts. It is quite reasonable to consider the last two compartments as one, thus simplifying the analysis via a two compartmental model. Figure 3 shows graphically the two compartments. It should be noted that CO_2 from the blood is transferred to alveoli with a rate coefficient k , but also (not necessarily at the same time) some of the agent in the alveoli is fed back into blood. This feedback is an important process in the analysis. Blood (the rapid exchange compartment) is a complex one, exchanging its content with other compartments leading to an assumption that blood is a vehicle by which the effect of ingested CH_3HgCl is superimposed on all other peripherals, thus influencing the ^{14}C excretion pattern. The excretion from the blood pool is not linear in nature, thus the solution to the kinetics is not known (Piotrowski, 1971, pp 9-22), but it is probable that at some point in time there will be an equilibrium during which the rate of excretion of ^{14}C from the blood is proportional to the concentration of ^{14}C in the blood. Thus, within this span of time blood can also be represented as a first order process (R. Aris, 1966). To make it right, however, the effect of other storage organs (liver, kidney, etc.) on the blood must be taken into account. If one considers the effect of all the storage organs collectively as one compartment, one obtains a fairly good model as shown in Fig. 4.

From Figure 4 we observe that the total amount of ^{14}C must be accounted for (preservation of matter) at every instant of time.

$$B + L + A + \Sigma O + F = \text{Constant} \text{ --------------- } (2)$$

Where B, L, A, ΣO and F are concentrations of ^{14}C in blood, lung, expired air, storage organs and excretion via feces and urine, respectively.

A System of differential equations that will satisfy this condition is as shown:

$$\frac{dB}{dt} = -(k_1 + k_4)\,B + k_6 L + k_8 \Sigma O$$

$$\frac{dL}{dt} = k_7 A + k_1 B - (k_6 + k_2)\,L = k_1 B - (k_6 + k_2) L$$

$$\text{since } k_7 \cong 0$$

$$\text{-------------- } (3)$$

$$\frac{dA}{dt} = k_2 L - k_3 A$$

$$\frac{d\Sigma O}{dt} = k_4 B - (k_8 + k_5)\,\Sigma O$$

At t = 0, ^{14}C is injected into blood, thus B(0) = 100% = constant C.

The four first order differential equations are reduced to one fourth order of the form:

$$\frac{d^4A}{dt^4} + \alpha \frac{d^3A}{dt^3} + \beta \frac{d^2A}{dt^2} + \gamma \frac{dA}{dt} + \Delta A = 0 \text{ ------ } (4)$$

The solution to the model is:

$$A = C_1 \text{ EXP } (-\lambda_1 t) + C_2 \text{ EXP } (-\lambda_2 t) + C_3 \text{ EXP } (-\lambda_3 t) + C_4 \text{ EXP } (-\lambda_4 t) \text{ ------------------------ } (5)$$

were A = amount of total injected, ^{14}C excreted in unit time

$\alpha, \beta, \Delta, \lambda_1, \lambda_2, \lambda_3, \lambda_4,$ = constant coefficients that depend on the animal and the toxic agent.

The initial conditions for the model require that at t = 0, A(o) = 0 therefore $C_1 + C_2 + C_3 + C_4 = 0$.

The model was tested against data from four experiments on an analog and digital computer. The system of data acquisition and curve fitting of model to the data is shown in Figure 5.

The analog computer program is shown in Fig. 6. The output of amplifier 10 is the solution to equation 5. The output from integrator 5 is the total cumulative value of ^{14}C-excreted, and its value at time t_1 is used to measure the severity of effect by comparing the values of the integral at t_1 between the control and the exposed animals.

In modeling the process on the analog computer, data mean values are plotted vs. time on a graph paper and the output from amplifier 10 is plotted (using x - y recorder) on the same graph. Rate coefficients represented by potentimeters (numbers in circles - see Fig. 6) are varied, until a fit is obtained. Typical output is shown in Fig. 7.

The total cumulative value of excreted ^{14}C is obtained from integrator 5 (Fig. 6). The result is an "S" shaped curve. By selecting a point in time t_1 (just before the saturation region) as a reference, the value of the integral at this point is used to compare control and exposed animals yielding a "yardstick of severity" of effect. Example is shown in Fig. 8.

The actual computation of effects for the four experiments has been done on a digital computer.

The results are tabulated in Table 1 and the closeness between the actual data and the simulated one is clear. Typical fit between data and the model is shown in Fig. 9 (control) and Fig. 10 (exposed), while the cumulative value computed is shown in Fig. 11.

Simplified Model

Although taking 8 measurements reduces the time required for the experiment, it still makes the method of prediction a tedious one. Real simplification is obtained if some approximation of the model is accepted. Models having two unknown coefficients can be developed that will provide same answers at time t_1 to that of the actual model. The simplified model is developed as follows:

As mentioned before, blood is a central compartment where mixing of a number of effects occurs. Mathematically this can be expressed as a multiplication. The proposed model is shown in Figure 12.

The decrease of ^{14}C in the blood (following injection) has a distribuion that decreases nonlinearily with time. By trial and error, an empirical function is suggested that offers a solution to the problem.

Assume the decrease with time of ^{14}C in the blood follows a distribution:

$$-\beta_1\ (1 - \frac{2}{1-\beta_1 t^2)}$$

where β_1 is a constant and t is the running time.

The output from the blood compartment is then equal to:

$$y^{11} = -\beta_1 t(1-\frac{2}{1\beta_1\ t^2})\ .\ y^1 \text{-----------------}(6)$$

Where y^1 = 1st derivative of $^{14}CO_2$ excretion

y^{11} = 2nd derivative of $^{14}CO_2$ excretion

Let $y^1 = p$

Then

$$\ln\ p = -\frac{1}{2}\beta_1 t^2 + \ln\ (1 - \beta_1 t^2) + \ln\alpha_1$$

where α_1 = integration constant

$$\text{and}\quad p = EXP\ (-\beta_1 t^2/2)\ \cdot\ 1-\beta_1 t^2\ \alpha_1 = y^1 \text{-----}(7)$$

Integrating equation 7 a distribution with time for the exhaled $^{14}CO_2$ is:

$$y = \alpha_1 t\ EXP(-\beta_1 t^2/2) \text{--------------------}\ (8)$$

with α_1 and β_1 being constant coefficients that are used in prediction of effects. Equation (8) satisfies all boundary conditions:

$t = 0 \qquad y = 0$

$t = \infty \qquad y = 0$

$t = \sqrt{1/\beta} \qquad y = max$

The model in eqn. 8 has only two unknown coefficients α_1, β_1 therefore taking two separate measurements at the beginning of the study, prediction can be made as to the effects at a later time. Using the model of eqn. 8, the four studies have been analyzed on the digital computer with results shown in Table 2. The closeness between the model of eqn. 3 and the model in eqn. 8 is self evident.

DISCUSSION

A mathematical model has been described that simulates the distribution with time of the $^{14}CO_2$ excretion from the lungs during the radiorespiratory experiment. The model described by eqn. 3 calls for 8 measurements during the early stages of the experiment. To simplify the matter, a simple model with only two coefficients is described in eqn. 8. To simulate the models, analog and digital computers have been used.

Although the analog method is sufficient to solve the problem and the value of α_1 and β_1 coefficients for each animal can be read directly from the settings of the coefficient potentiometers, a solution on digital computer has been sought. A digital computer provides the direct numerical values needed to answer the effects of a pollutant. The analog computer, however, permits a quick determination of the on-going process and also permits an instantaneous change of coefficients making it a flexible tool in the hands of a researcher.

In Tables 1 and 2, results from four experiments compared to the two model are presented. In particular, it can be seen that, up to time $t = t_1$, just before the saturation, the values for total excretion indicate a substantial decrease in the excretion in the exposed animals and that the correlation between the calculated values and the models is a readily acceptable one. These facts suggest that it is possible to predict biological effects of a pollutant or toxicant under specific conditions by simulation and interpolation on a computer.

TABLE 1. Comparison of Percent Cumulative Excretion Values Between Actual Experimental Data and Simulated Data

Group	No. of Animals	Calculated Cumulative Value in % Using Data t_1 = 145 min.				Cumulative Value in % Using Model t_1 = 145 min.			
		Control	Exposed	Δ	%Δ	Control	Exposed	Δ	%Δ
A	4	65.08	61.64	3.43	5.20	66.17	50.56	5.61	8.47
B	4	71.04	48.577	22.46	31.6	72.50	49.00	23.50	32.41
C	4	61.56	55.97	5.6	9.01	62.95	57.74	5.21	8.27
D	4	66.17	60.27	5.9	8.92	65.21	58.4	6.8	10.5

Table II. Comparison of Percent Cumulative Excretion Values Between Actual Experimental Data and Simulated Data By the Simplified Model

Group	No. of Animals	Calculated Cumulative Value in % Using Data t_1 = 145 min.				Cumulative Value in % Using Simplified Model t_1 = 145 min.			
		Control	Exposed	Δ	%Δ	Control	Exposed	Δ	%Δ
A	4	65.08	61.64	3.43	5.20	62.7	59.5	3.2	5.10
B	4	71.04	48.577	22.46	31.6	71.34	47.05	24.29	34.00
C	4	61.56	55.97	5.6	9.01	61.64	56.145	5.50	8.90
D	4	66.17	60.27	5.9	8.92	66.175	58.87	7.30	11.03

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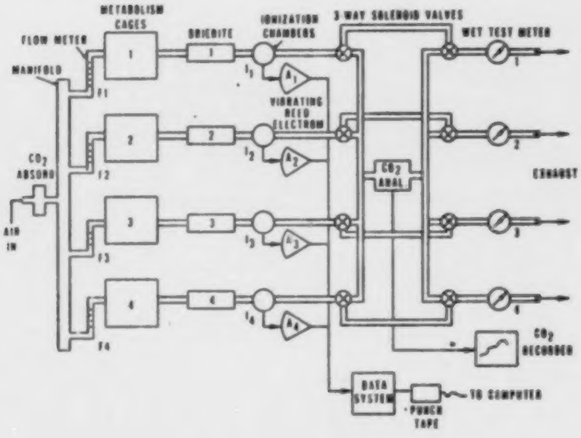
METABOLISM CAGES
FLOW METER
MANIFOLD
DRIERITE
IONIZATION CHAMBERS
3 WAY SOLENOID VALVES
WET TEST METER
VIBRATING REED ELECTROM
CO_2 ABSORB
AIR IN
F1
F2
F3
F4
I_1
I_2
I_3
I_4
A_1
A_2
A_3
A_4
1
2
3
4
CO_2 ANAL
EXHAUST
CO_2 RECORDER
DATA SYSTEM
PUNCH TAPE
TO COMPUTER

Figure 1. Flow System and Instrumentation Block Diagram for Radiorespirometry

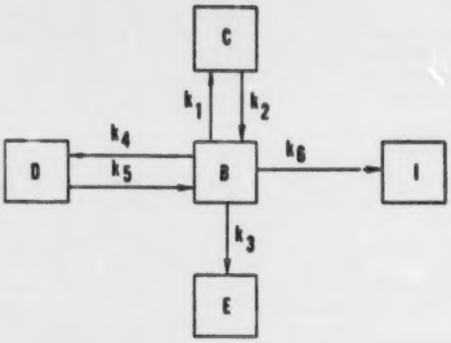
C
D
B
I
E
k_1
k_2
k_3
k_4
k_5
k_6

Figure 2. Generalized Kinetic Model for Transfer Process of an Agent from Blood to Other Parts of the Animal's Body

B = Agent in the blood

C = Agent in fast exchange organs

D = Agent in slow exchange organs

I = Agent removed "irreversibly" from lungs

E = Agent excreted by urine and feces

k_1, k_2, k_3, k_5, k_6 = Rate coefficients; and depending on the agent, k_4 and $k_5 \geq 0$

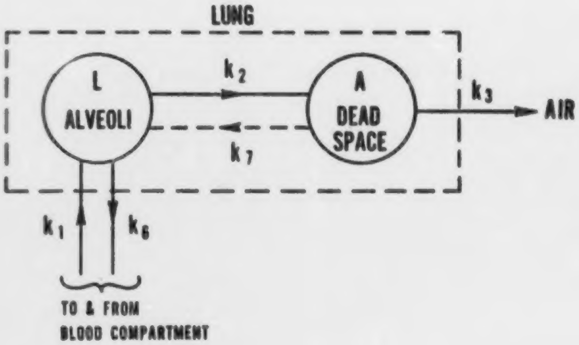
LUNG
L
ALVEOLI
A
DEAD SPACE
k_2
k_7
k_3
AIR
k_1
k_6
TO & FROM BLOOD COMPARTMENT

Figure 3. Lung System Represented by Two Compartments

L = Alveoli compartment

A = "Dead space" compartment

k_1, k_2, k_3, k_6, k_7 = Rate coefficients of agent excreted to and from compartments

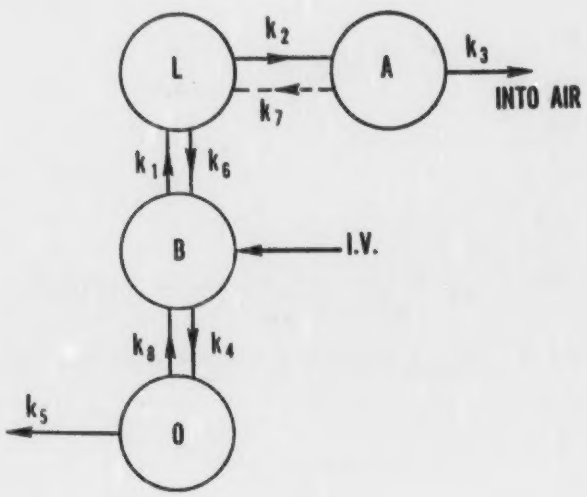
L
k_2
A
k_3
INTO AIR
k_7
k_1
k_6
B
I.V.
k_8
k_4
k_5
0

Figure 4. Model for Blood Lung Interaction

B = Agent level in the blood

L - Agent level in the alveoli

A = Agent level in the "dead space"

ΣO = Agent in other organs (liver, kidney, etc.)

k_1, k_2, k_3, k_4 = Rate coefficients of excretion from a compartment

k_6, k_7, k_8 = Rate coefficients of excretion returned to a compartment

k_7 = Coefficient of return rate from "dead space" to alveoli = 0

k_5 = Rate coefficient of excretion of irreversibily removed agent by urine and feces

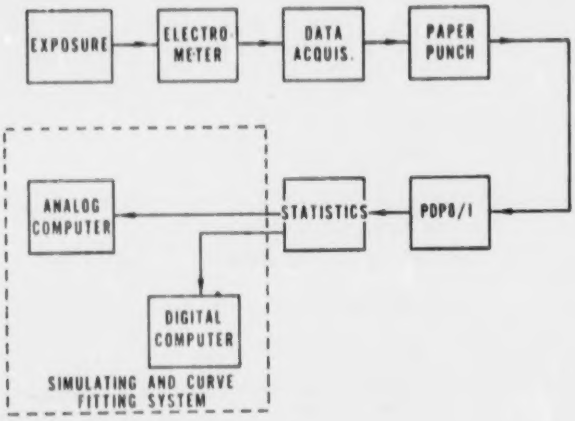
EXPOSURE
ELECTRO METER
DATA ACQUIS.
PAPER PUNCH
ANALOG COMPUTER
STATISTICS
PDP8/I
DIGITAL COMPUTER
SIMULATING AND CURVE FITTING SYSTEM

Figure 5. System Flow Diagram for Data Acquisition and Curve Fitting of Model to Data

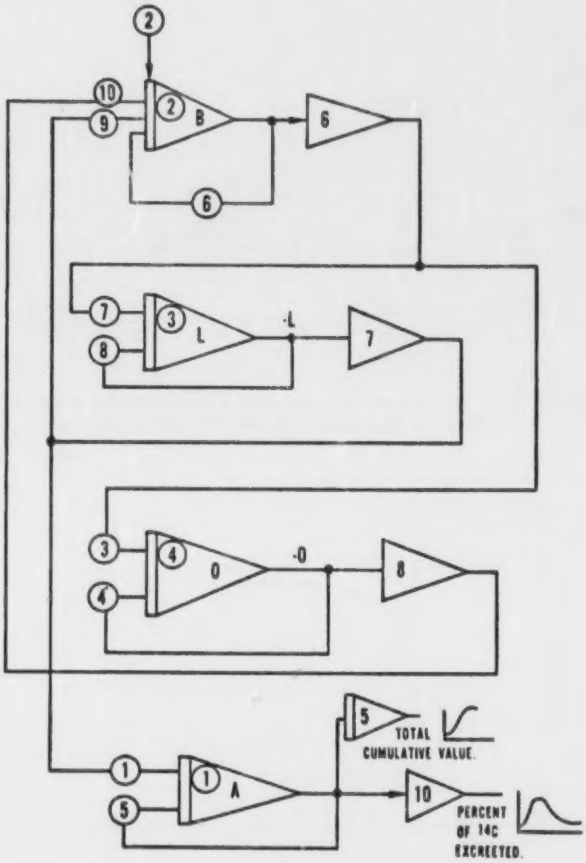
2
10
9
2
B
6
6
7
8
3
L
-L
7
3
4
4
0
-0
8
5
TOTAL CUMULATIVE VALUE
1
5
1
A
10
PERCENT OF 14C EXCRETED

Figure 6. Analog Computer Program for the Model of $^{14}CO_2$ Excreted from the Lungs

Integrator B = Blood compartment

Integrator L = Alveoli compartment

Σ O = Compartment representing other body organs

A = "Dead space" compartments

6, 7, 8, 10 = Amplifiers

5 = Integrator producing total cumulative value of excreted ^{14}C

Numbers in circles represent rate coefficients

② = Initial condition (I.V. injection)

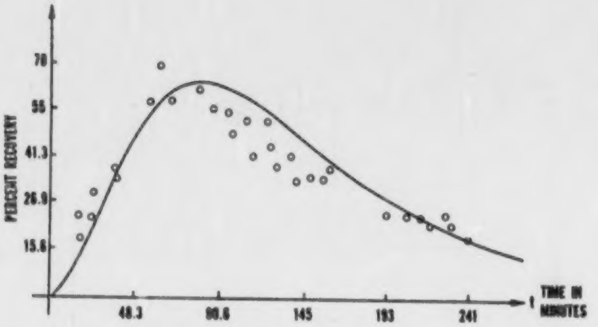

Figure 7. Comparison Between the Curve Generated by the Analog Computer and the Experimental Data

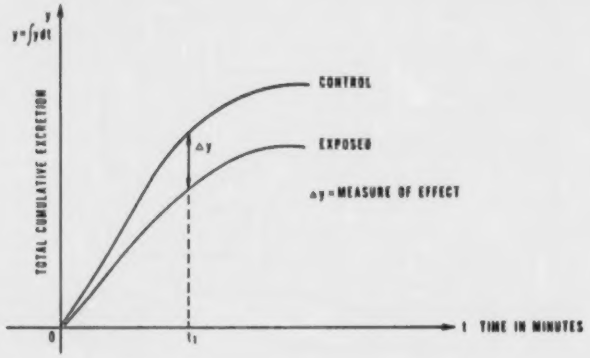

Figure 8. Example of a Total Cumulative Excretion Curve for a Control and Exposed Animal

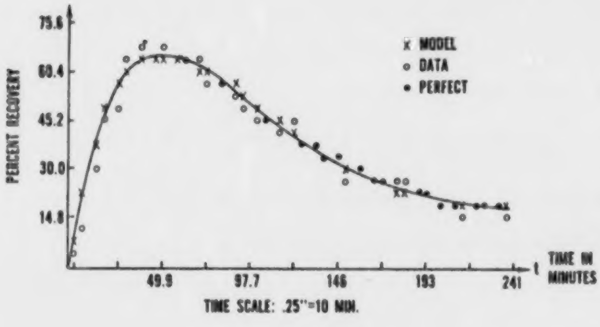

Figure 9. Curve Fitting Between Experimental Data and the Model of Group B - Control

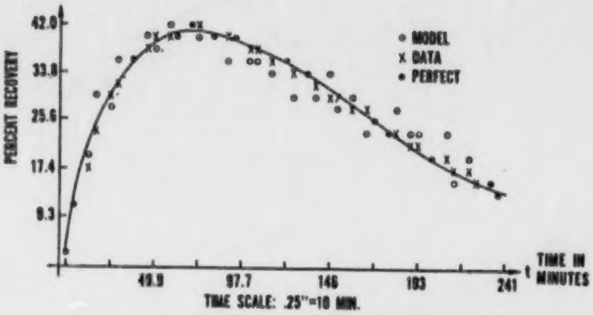

Figure 10. Curve Fitting Between Experimental Data and the Model of Group B - Exposed

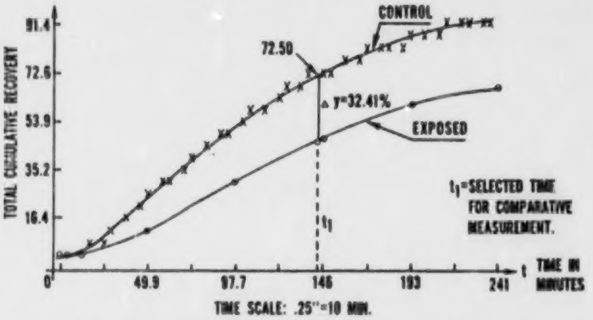

Figure 11. Total Cumulative Recovery for Control and Exposed Group A

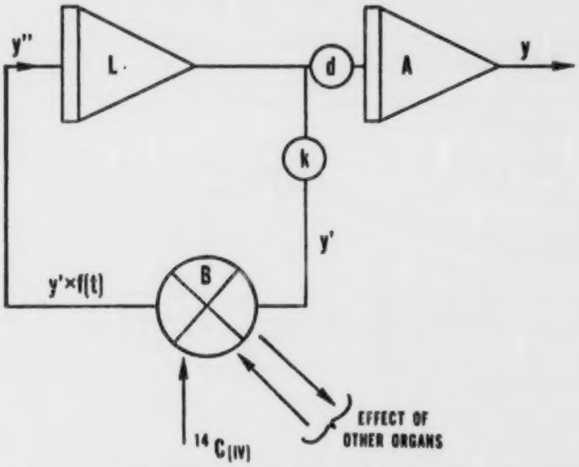

Figure 12. Simplified Kinetic Model for Transfer Process of an Agent from Blood to Lungs

y = Percent of ^{14}C excreted in unit time

y^1 = First derivation of y

y^{11}, = Second derivation of y

k, d = Constant rate coefficients that depend on the process

I.V. ^{14}C = I.V. injection of ^{14}C into blood

B = Blood compartment (multiplier)

L = Alveoli compartment

A = "Dead space" compartment

ESTIMATION OF THE OPTIMAL SAMPLING INTERVAL IN ASSESSING WATER QUALITY OF STREAMS

Leo J. Hetling, G.A. Carlson and J.A. Bloomfield
Environmental Quality Research Unit
New York State Department of Environmental Conservation
50 Wolf Road, Albany, New York 12233

The problem of estimating the sampling resources necessary to characterize water quality is one that has received little attention. Until recently, the problem was unimportant because the resources available for monitoring were limited and the thrust of most programs was not so much to characterize the system as to detect specific violations of a set water quality standard. Recently, however, the resources available for monitoring of the environment have been increasing and a determination of optimum utilization of these resources becomes of practical significance. Additionally, the progress made in point source pollution control has led to greater emphasis on non-point source pollution problems. Non-point source problems require a more detailed knowledge of annual and seasonal loadings rather than measurement of deviation from a standard.

The problem most often encountered is to develop a sampling strategy for statistical characterization of the concentration and annual loading of a pollutant from a watershed. Most existing monitoring programs are set up such that chemical samples of a stream are collected at fixed sampling intervals; i.e., weekly, bi-weekly, monthly, etc. Stream flow at the point and time of sampling is noted. Average annual concentrations and loadings are then calculated from this data base. Although the limitations of this approach have been recognized, little analytical or experimental work has been done to document errors involved with the strategy.

We first attempted to approach the problem analytically. However, it was found that since neither stream flows nor concentrations are normally distributed, attempts at analytical solutions were frustrating. As a result, the following more experimental approach was pursued. A continuous stream flow gage was installed on a small stream and grab samples for water quality were collected daily. Using equally-spaced subsets of the resulting data set, average concentrations and loadings were calculated and compared to the average obtained by utilizing the entire data set. This approach was first suggested by Treunert, _et al_ (1); however, his analysis was limited in that concentration measurements available to him were spaced at three-day intervals.

Mill Creek, the stream utilized for this study, is a small stream draining 2,454 ha in Rensselaer County near Albany, New York (Figure 1). The land use in the watershed is predominantly forest (54%) and agriculture (43%). The stream is unregulated and has no known point sources of pollution. A complete description of this watershed is available (2). Stream flow was measured via a standard stage height recording station installed, rated and maintained by the United States Geological Survey. Chemical samples were collected, preserved and delivered to the New York State Department of Health's Division of Laboratories and Research for analysis. The actual chemical analyses performed are described in Krishnamurty and Reddy (3). This paper utilizes 275 daily samples taken from March 1, 1975 through November 30, 1975.

Twenty water quality constituents were analyzed including major ions and the various forms of carbon, nitrogen and phosphorus. This paper will concentrate on elucidating the effect of sampling interval on the estimation of the average daily concentration and average instantaneous load of total suspended solids (retained on a 0.45 μ filter), chloride and particulate and dissolved phosphorus.

The average daily concentrations ($\bar{C}$) and the average daily loadings ($\bar{L}$) were calculated for subsets of the data taken at fixed intervals ranging from one to 60 days. Sampling frequencies of longer than two months were considered to be random rather than fixed-interval sampling and hence ignored. Ten sample populations of 265 days length were withdrawn from the general population by beginning fixed interval sampling on each of the first ten days of the sample space (Sample $\equiv$ March 1, 1975) (Figure 2). The average concentration is defined as follows:

$$\bar{C}j,m = \frac{1}{n} \sum_{\substack{i = j \\ \text{by } m}}^{j+s-r} Ci \qquad (1)$$

where:

$$n \cong \frac{s - r + m}{m} \qquad (2)$$

and

n = number of samples in each discrete population
j = the initial sample chosen (March 1 $\equiv$ 1, $1 \leq j \leq r$)
m = imposed sampling interval ($1 \leq m \leq 60$ days)
s = total number of samples in the general sample space = 275
r = number of discrete populations withdrawn from the general sample space (10)
Ci = constituent concentration (mg/l) on the ith day
$\bar{C}j,m$ = arithmetic average concentration (mg/l) calculated beginning on the jth day at an interval of m days

It should be pointed out that the number of samples (n) in each withdrawn population is not identical for a fixed interval. The explanation is that a few of each of the chemical analyses were considered as "suspicious" by field and laboratory personnel and these data were not utilized in the statistical treatment. Thus, this discussion and analysis considers that the average surveillance scheme will result in a small number ($<$5%) of "missing" values.

The equation for average instantaneous daily loading is:

$$\bar{L}j,m = \frac{8.64}{n} \sum_{\substack{i=j \\ \text{by } m}}^{j+s-r} Ci \cdot Qi$$

where:

Qi = instantaneous flow at the time of collection of the ith sample (m3/sec)

$\bar{L}j,m$ = the arithmetic average daily loading calculated beginning on the jth day at an interval of m days (Kg/day)

The results of the calculations are shown in Figures 3 through 6. The abscissa of these plots is the imposed sampling frequency; i.e., daily, every other day, weekly, every third day, etc. On the ordinate, the average of the ten data sets obtained for imposed sampling frequency along with the range of values observed was plotted. As a reference, the average value obtained utilizing the entire data set is shown along with lines showing a 25, 50 and 75% deviation from this value.

All of the plots have several characteristics in common. The range of values spreads rather rapidly as the sampling interval is increased. This rapid deviation is to be expected since the number of samples within a data set decreased rapidly as the sampling interval is increased. This is illustrated in Figure 7 where the number of samples from the 275 sample data sets obtained is plotted against the sampling frequency.

The rate at which the range increases varies with the parameter being studied. It is least rapid for the chlorides (a dissolved, conservative ion), more rapid for dissolved phosphorus which takes part in a variety of chemical sorption, and exchange reaction with the stream bed and surrounding soils, and most rapid for the particulate-related parameters of suspended solids and particulate phosphorus.

A wider band of errors can be noted for loading than for the concentration values.

It is apparent from these plots that unless one samples very frequently (at least every other day), average values calculated from the data can range considerably from the actual daily average. Frequent sampling is of even more importance with the particulate-related material where order of magnitude errors could be encountered with less than a three-day sampling frequency.

A tendency for the average value to decrease as sampling frequency is increased is also noted for the particulate parameters. Apparently as the sampling frequency decreases, the likelihood of sampling the major stream flow events also decreases. Since extreme events have a profound effect on averages, a value somewhat less than the average obtained by utilizing all of the data is obtained. This indicates that as sampling frequency decreases, there will be a tendency to underestimate the actual average concentrations and loadings for particulate material.

Conclusions

As a result of this analysis, it can be concluded that for small streams similar to Mill Creek, fixed interval sampling to obtain average concentrations is of little value unless the sampling interval is less than two or three days. Attempts to obtain annual loads are even less productive unless daily or every other day samples are taken.

Apparently this occurs because of the importance of a relatively few major hydrological events on the annual average. Hopefully, a sampling strategy centered around these events can be devised to obtain reasonable estimates of average concentrations and yield without the extreme investment needed for daily sampling.

Future plans of this study are to repeat the above and similar analyses utilizing a full year's worth of the Mill Creek data. A greater number of parameters will be studied and the effect of utilizing the continuous stream flow record with fixed interval chemical quality sampling will be investigated. The effectiveness of various event sampling strategies will also be tested.

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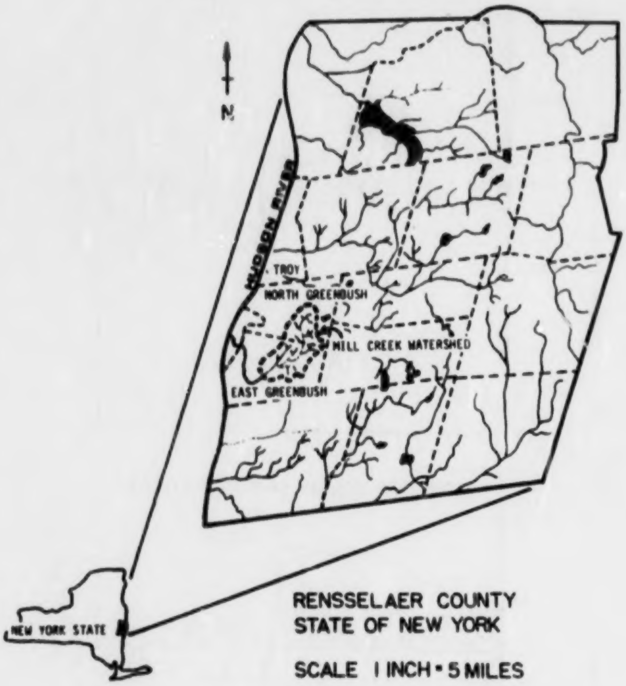
N
HUDSON RIVER
TROY
NORTH GREENBUSH
MILL CREEK WATERSHED
EAST GREENBUSH
NEW YORK STATE
RENSSELAER COUNTY
STATE OF NEW YORK
SCALE 1 INCH = 5 MILES

FIGURE 1.

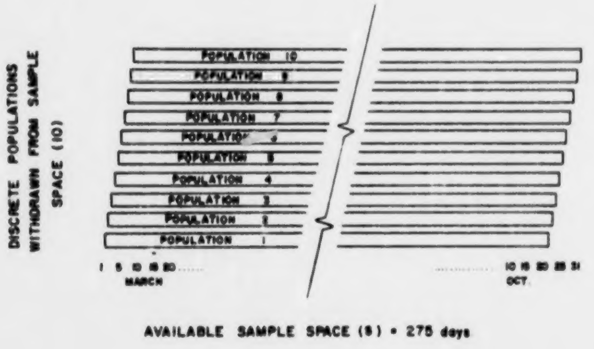
DISCRETE POPULATIONS WITHDRAWN FROM SAMPLE SPACE (10)
POPULATION 10
POPULATION 9
POPULATION 8
POPULATION 7
POPULATION 6
POPULATION 5
POPULATION 4
POPULATION 3
POPULATION 2
POPULATION 1
1 5 10 15 20
MARCH
10 15 20 25 31
OCT.
AVAILABLE SAMPLE SPACE (S) = 275 days

FIGURE 2.

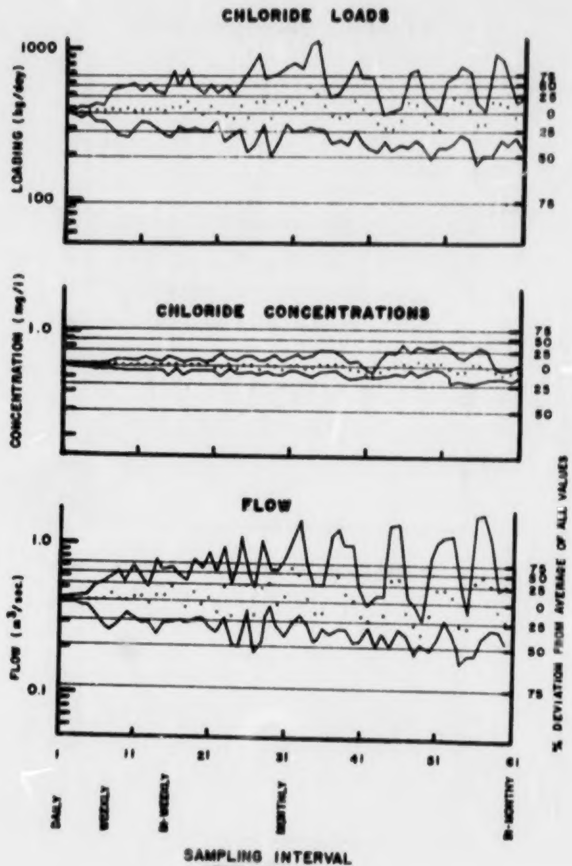

FIGURE 3.

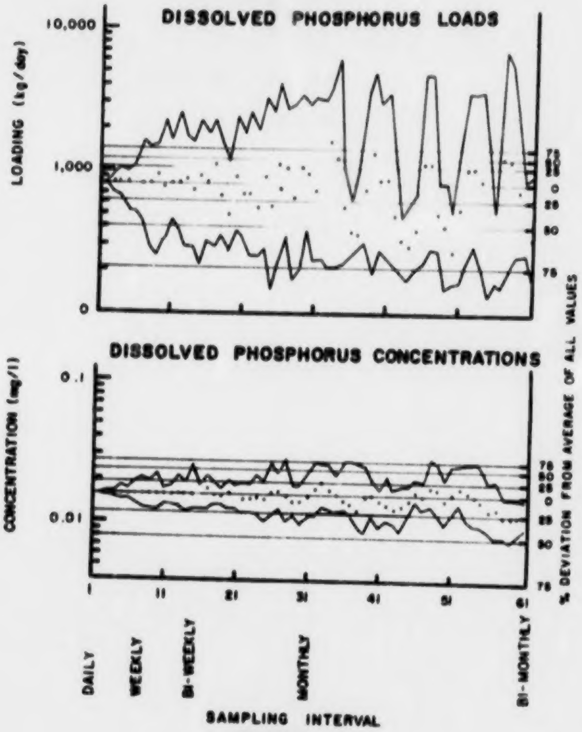

FIGURE 4.

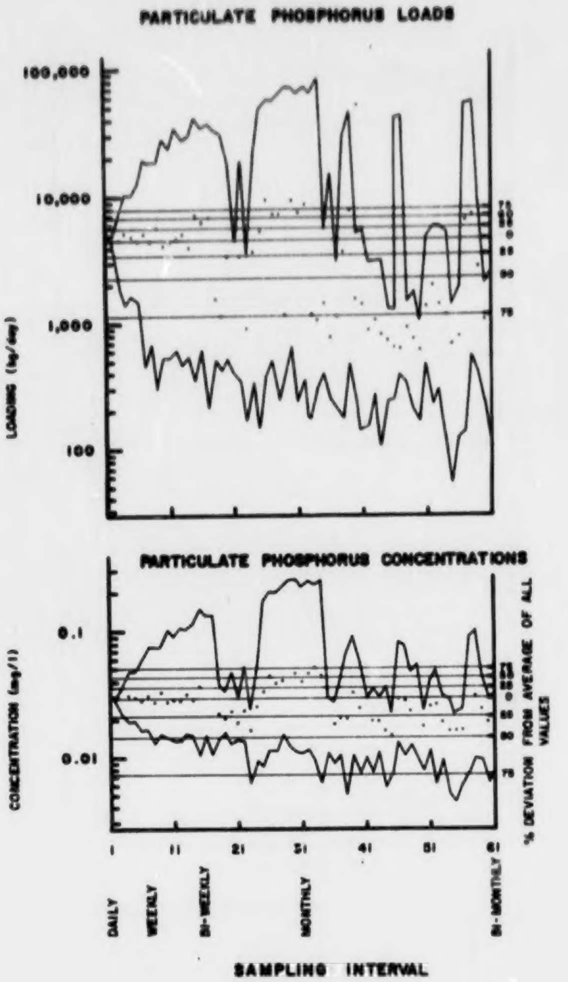

FIGURE 5.

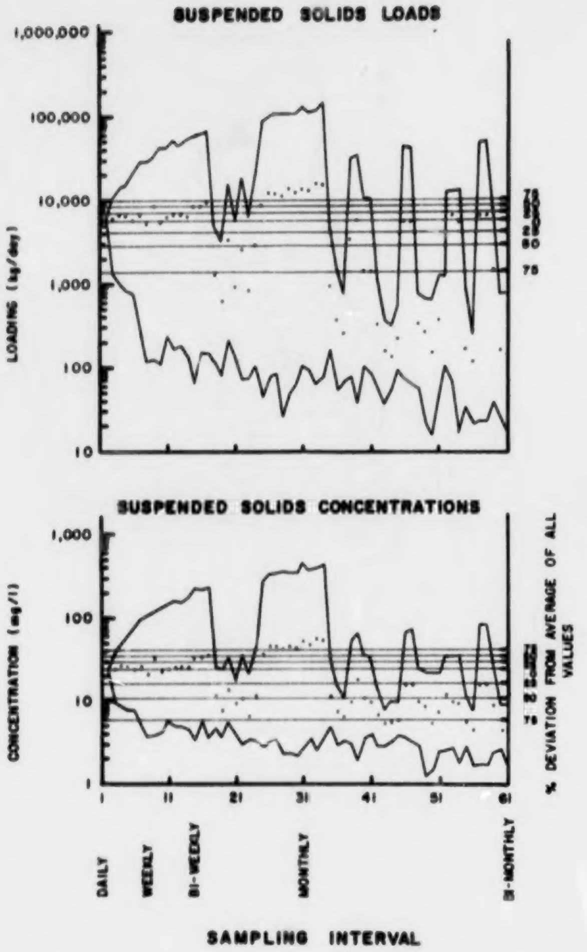

FIGURE 6.

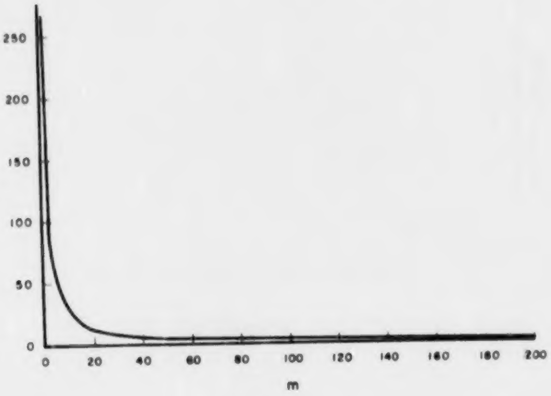

FIGURE 7.

FIELD DATA FOR ENVIRONMENTAL MODELING—ADJUNCT OR INTEGRAL?

Philip E. Shelley, PhD
Director, Energy and Environmental Systems
EG&G Washington Analytical Services Center, Inc.

Summary

Two types of field data are required for virtually all environmental prediction models: calibration data and verification data. The former type is used within the model itself to ready it for specific application, whereas the latter is used to establish the validity and probable accuracy of the results obtained from the model. The paper points out that, historically, too little attention has been given to the collection of field data for use with environmental models and that the quality of the current modeling state-of-the-art generally far exceeds the quality of the supporting data base. An incredible lack of good data faces the model developer, evaluator, and user alike, and this often unrecognized fact quite seriously impacts on the activities of each. Using urban hydrology models as an example, the severity of the problem is demonstrated. The need for determining estimates of data quality prior to their use in modeling is noted, and the dangers associated with the "blind" use of existing data are indicated.

Introduction

adjunct (aj'u͡ng kt) 1. something added to another thing but not essentially a part of it.

integral (in'tə grəl) 1. of, pertaining to, or belonging as an essential part of the whole.

Environmental modeling is performed in order to obtain a picture of probabilistic events likely to occur given a set of input conditions. The "portrait" obtained will be of the right "person", but even a charicature can be useful in many instances, despite its exaggerations, as long as it is recognizable. Regardless of whether the application arises from the needs of planning, design, facility operation, alternative assessment, or other needs, the simulation process involved is intended to duplicate the essence of a system without actually attaining reality itself; the model is simply a device used to carry out the simulation. The validity of the results, i.e., their agreement with reality, depends upon two primary factors: how well the model represents the actual processes involved, and how representative the set of input conditions are. In general, both of these factors involve the use of field data and, for any given model, the better (i.e., more realistic/representative the field data, the closer the simulation will be to reality. Although the following is drawn from the field of urban hydrology, most of what is stated essentially applies to other environmental modeling areas as well.

Regardless of whether the model of interest is stochastic versus deterministic on the one hand, or analytic versus synthetic on the other, there are two uses that are generally made of field data. To emphasize the importance of distinguishing between the two, they will be referred to here as data types. Because of the complexity of the processes being modeled, most of the models that are popular today require field data both for estimating empirical parameters in their structure and for fitting other application-specific parameters (calibration). For example, one version of the Sanford Watershed Model has twenty parameters: two are based on meteorological data, four are based on hydrograph separation, five are computed from physical measures, three are estimated from empirical tables, and six are fitted. All field data that are used within any model structure, i.e., to ready the model for specific application, will be referred to here as calibration data.

The chief concern of the model-user is how well the model outputs (which are its sole reason for being) compare to reality. This comparison forms a measure of the predictive capability of the model. Here, also, input and output field data are required, but their fundamental use is quite different from that of calibration data. They will be referred to here as verification data, since they are used to verify the results of a particular model exercise.

This distinction between field data types is not made to suggest that different gathering techniques are required for calibration versus verification data; in fact, they are the same. The reason for making the distinction is simply that calibration data must never be used for model verification. The importance of this simple statement cannot be overestimated.

Data in Model Selection

The various stormwater management models that are available today require data on the catchment, precipitation, and runoff quantity and quality. Such data might include historical and current records plus related information such as present and projected land use parameters, demographic projections, remote (satellite or aerial) imagery, treatment plant records, and the like.

The purpose of the simulation, i.e., the use to which the model results are put, must be kept in mind in selecting the model to be employed, but it is also very important to carefully review and inventory the existing data base. As Lager has noted, "Rather than selecting a model and then seeing if you can fill its data requirements, it is preferable to analyze your available data and then choose the model that can use these data most effectively to achieve study objectives."[1]

The various models not only have different basic data requirements; they also vary widely in the detail of temporal and spatial distribution of data required. For example, some models require time steps of less than one minute to satisfy numerical stability conditions, while others can be run with hourly, daily, and even up to semimonthly data. These considerations, with their attendant field data gathering cost implications, bear heavily on model selections.

Considerations other than the model structure are also involved in determining the cost of a field data gathering program. For example, both the quantity and quality of stormwater runoff are highly variable and transient in nature, being dependent upon meteorological and climatological factors, topography, hydraulic characteristics of the surface and subsurface conduits, the nature of the antecedent period, and the land use activities and housekeeping practices employed. It is this highly variable and transient nature of stormwater flows that makes their characterization so difficult and, hence, expensive. In addition to tremendous dynamic ranges, the poor quality of stormwater draining from the urban environment has a significant effect on the choice of suitable sampling and flow measurement equipment and methods as well as an impact in the analytical laboratory.

Data Quality

In addition to assessing the quantity of data on hand and to be gathered, some assessment of data quality is required if we are to be sure that our "portrait" is of the "right person." We are not yet overwhelmed with existing data on stormwater characteristics. As stated by Torno, "One of the serious problems that faces either a new model developer or one who must evaluate several models is the incredible lack of good data..."[2] To be effectively utilized, we need more than simple values as data products. We need to know something about the data quality, i.e., about the "goodness" or truthfulness of the data. Two terms that relate to the data-gathering process are conventionally used to describe data quality: accuracy and precision. Accuracy refers to the agreement between the measurement and the true value of the measurand, with the discrepancy normally referred to as error; precision refers to the reproducibility (repeatability) of a measurement when repeated on a homogenous time-stationary measurand, regardless of the displacement of the observed values from the true value, and thus, indicates the number of significant digits in the result. We are, therefore, interested in establishing the best estimate of a measured quantity and the degree of precision of this estimate from a series of repeated measurements. Calibration, whether it be of a piece of flow measurement equipment, a chemical method for wastewater analysis, or a stormwater management model, is simply the process of determining estimates of accuracy and precision.

Discrepancies between the results of repeated observations, or errors, are inherent in any measurement process, since it is recognized that the true value of an object of measurement can never be exactly established. These errors are customarily classified in two main groups: systematic and random (or accidental) errors. Systematic errors usually enter into records with the same sign and frequently with either the same magnitude (e.g., a zero offset) or with an establishable relationship between the magnitude of the measurement and the error. The methods of symmetry and substitution are frequently used to detect and quantify systematic errors. In the method of symmetry, the test is repeated in a symmetrical or reversed manner with respect to the particular condition that is suspect. In the method of substitution, the object of measurement is replaced by one of known magnitude (a calibration standard), an instrument with a known calibration curve is substituted for the measuring instrument in question, and so on. Thus, systematic errors bear heavily on the accuracy of the measurement.

Random errors, on the other hand, are due to irregular causes, too many in number and too complex in nature to allow their origin to be determined. One of their chief characteristics is that they are normally as likely to be positive as negative and, therefore, are not likely to have a great effect on the mean of a set of measurements. The chief aim of a data quality assurance effort is to account for systematic errors and thereby reduce errors to the random class, which can be treated by simple probability theory in order to determine the most probable value of the object of observation and a measure of the confidence placed in this determination.

The statistical measures of location or central tendency (e.g., the various averages, mean, median, mode) are related to accuracy. The statistical measures of dispersion or variability (e.g., variance and standard deviation, coefficient of variation, and other measures derived from central moments of the probability density function) are related to precision.

There are also some annotations that the data gatherer can make to increase the usefulness of the data. For example, inspection of equipment and records may indicate periods of instrument malfunction or failure (e.g., power interruptions). These facts are important and should form a part of the total record. There may be circumstances discovered during site visits that would have had an effect on preceding data that cannot be readily determined, e.g., a partially blocked sampler intake or a rag caught in the notch of a weir. These facts should also be noted and, where at all feasible, some qualitative notation as to expected data quality (e.g., poor or very good) should be made.

The importance of notations of data quality results from the ultimate use of the data. For example, at the risk of seeming ridiculous, ±50-percent data should not be used to calibrate a model whose outputs are desired within ±20 percent, nor should strong model verification judgments be made based upon a very small sample of data with a high variability. The levels of data quality desired vary with the intended use of model outputs. The needs for overall basin planning, treatment plant design, plant operation, and research are all quite different, and this must be kept in mind in designing the data-gathering program (or system).

Instrumentation

The ability of available instrumentation and techniques to gather reliable wastewater characterization data varies widely with design and implementation factors. Shelley has reviewed the sampling problem[3,4] and has collected comparative data using various samplers.[5] Shelley and Kirkpatrick have recently provided in-depth monographs on instrumentation for flow measurement[6] and sampling.[7] A summary of the use of instrumentation for collecting field data for stormwater model calibration has been given by Shelley.[8] who has also examined the use of remote sensor data to measure water quality, especially sediment.[9]

To summarize the foregoing as it pertains to stormwater flow measurement, it can be stated that, although accuracies on the order of ±5 percent can be achieved with the proper site, instrumentation, and care, instrument readings that differ from spot checks by 25 to 50 percent or more are much more typical. There are a number of factors involved, but the greatest contributor seems to be the use of slope-area methods such as the Manning formula in uncalibrated reaches or inappropriate instances.

Reviews of project experience have revealed cases where individual meters have been in error by over 200 percent, due to lack of proper maintenance, installation errors, or misapplication.

Insofar as sampling is concerned, the lack of a manual sampling protocol has resulted in a situation where differences of as much as 150 percent have been observed between samples taken manually from the same source at the same time, the differences being attributable to equipment and technique. In a recent side-by-side test of four different automatic sampler designs, a controlled synthetic waste stream was employed.[5] The results of laboratory analyses of samples taken with these equipments ranged from understatements of pollutant concentrations by 25 percent or more to overstatements by as much as 200 percent and higher. Again, a number of factors are involved, but equipment design characteristics (especially intake and sample-gathering subsystems) appear to account for much of the observed performance variation.

As regards chemical methods for the analysis of water and wastes, the picture is relatively brighter. Even here, the lack of well-accepted baseline standards or alternate techniques results in an inability to speak of accuracies for a number of tests. Furthermore, precision expressed as standard deviation is not outstanding for some tests. As an example, USEPA[10] quotes the results of 86 analysts in 58 laboratories who analyzed natural water samples plus an exact increment of biodegradable organic compounds. At a mean value of 175 mg/l BOD, the standard deviation was ±26 mg/l (±15 percent). For other tests, especially at low levels, even larger variances may be encountered.

When the foregoing sources of error are combined, for instance, as is necessary if mass discharges are to be computed/predicted, the picture is not very optimistic. Straightforward calculation shows that results can vary by over an order of magnitude; hardly a comforting situation for model calibration or verification. Along the same line, Harris and Keffer,[11] as a result of extensive comparative testing in the field, have noted that apparent treatment plant efficiencies can be varied by a factor of 2 or 3 or even higher, depending upon site selection and equipment used.

Conclusion

Although it was strongly implied earlier that field data should be viewed as integral to environmental modeling, the present state of affairs suggests that such data have been treated as adjunct in terms of the effort and resources that have been applied to the development and refinement of computer models vis-à-vis that devoted to the collection of good field data. This observation is not meant to suggest that all work on model refinement and use should be abandoned for a massive data-gathering expedition, but rather that we must bring our application of resources for environmental characterization/prediction into better balance. Obviously, much remains to be done in terms of refinement of equipment and techniques before our field data are up to the sophistication of some of our models, and it is past time that this fact be more widely recognized.

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DATA DEFICIENCIES IN ACID MINE DRAINAGE MODELING

Vincent T. Ricca, Ph.D.
Professor
Department of Civil Engineering
The Ohio State University
Columbus, Ohio

ABSTRACT

Recently developed digital computer models for Acid Mine Drainage Quality and Quantity for discharges from deep mines, strip mines, and refuse piles are currently being validated by application to field sites. A task in this current research was to select suitable test sites with extensive hydrologic and acid mine drainage data. Experience has shown that data for the some 200 modeling parameters as well as the length and consistency of the records have not been satisfactorily collected in the past on even the most highly investigated study sites. The object of this paper is not to criticize these prior collection efforts, for some were quite extensive indeed; but rather, to indicate what data should be collected if acid mine drainage modeling is to be advanced.

BACKGROUND

Over the past five years, researchers at The Ohio State University have been developing computer models to describe the quantity and quality generation of coal mine drainage. A two-year, EPA-sponsored research project titled, "Resource Allocation Model to Optimize Mine Pollution Abatement Programs"[1] was completed in 1974. A major component of the work in that project was the development of unit source models. These models predict the mine drainage flow and its associated acid load for deep or drift mines, strip mines, and refuse piles. They were created by combining highly sophisticated hydrologic simulation models and mine acid production models developed by the acid mine drainage task group at The Ohio State University. The outcome of this initial work on these unit source models is deemed quite successful and encouraging by the researchers involved. An objective of this original work was to produce models as detailed and sophisticated as possible, using the highest level currently available in the fields of hydrologic simulation and mine acid production. This approach was taken with the belief that it is a more feasible future task to simplify these highly detailed models than to upgrade simplistic models as field applications disclose the nature and availability of data involved in the phenomenon of acid production and mine discharges. Details of the basic unit source models are discussed in the final report of the model development project[1].

A follow-up EPA project[2] is currently nearing completion. An objective of this latter project is to apply the previously developed models to field situations to evaluate their validity. These applications provide information for another project objective: "Identifying Data Deficiencies and Formulate Data Acquisition Guidelines". This last objective will be the subject of this paper.

DISCUSSION OF THE DATA NEEDS OF THE MODELS

The unit source models are considered as highly sophisticated in their structure and performance. They are capable of producing continuous time outputs of generated mine site discharges and attendant acid quality of the flows as well as receiving stream or basin outlet flows. In order to accomplish this continuous time trace throughout the modeling period it is necessary to have compatible detail and consistency on the climatic input data. Also,much detail is needed on the physical and chemical aspects of the mines and spoils along with the site watershed. Some 200 parameters in total may be involved in a modeling endeavor depending upon degree of detail desired.

The listing below is a category description of the major information items, or input, required to operate the models. Explicit details on the input data and model parameters are given in the technical discussion of the model found in the project report.[1]

Basin Information. Watershed drainage, Land use and distribution, Flow capacity of main channel, Mean overland flow path length, Retardance coefficient for surface flows, Average ground surface slopes, Interflow and baseflow recession constants, Channel routing parameters, and Index parameters reflecting interception, depression storage, infiltration, soil moisture storage, interflow movement, groundwater movement, etc.

Climatic Data. Precipitation records, Streamflow records, Evaporation rates and coefficients, and Meteorological information for snowmelt.

Deep Mine Information. Mine area; Coal seam description, materials, thickness; Pyrite oxidation rate parameters reflecting diffusion, reaction, and temperature; Acid transport parameters reflecting gravity diffusion, inundation, and leaching; Initial acid storages; and Alkalinity conversion factors.

Refuse Pile-Strip Mine Information. Strip mine and refuse pile areas; Representative soil profiles of acid producing areas; Pyrite oxidation rate parameters reflecting diffusion, reaction, and temperature; Initial acid storages; and Acid transport mechanism parameters reflecting depth leached by direct runoff, leaching parameters, effective acid solubilities.

Discharge Data. Drainage flow records; and Drainage quality records.

SELECTION OF TEST SITES

In order to validate the unit source models, field or "test sites" were sought. Those working in the area of acid mine drainage and related coal mining problems are aware that many reports on demonstration projects and mining operations are available in the literature. Project researchers at OSU were aware of such literature and expected to find numerous "test sites" upon which to apply the models. However, once into this task, a wealth of information was found; but, consistency or completeness immediately surfaced as a major problem. To properly assess the possible test sites a systematic evaluation or selection methodology was developed. A discussion of this methodology follows.

The Nature of the Literature Review for Site Selection. Since this project is concerned with testing of the models, it is important to find the best possible watersheds, that is to say, the watersheds with the largest amount of available field data to use in the models. This requires the best streamflow records, stream quality records, meteorological and physical data that can be obtained, thus eliminating as many sources of error as possible. The researchers reviewed 40 separate reports concerning 33 watersheds. The majority of these reports were prepared by private consulting firms as a part of "Operation Scarlift" which was funded by the Department of Mines and Mineral Industries, Pennsylvania. Other sources of literature were EPA demonstration projects, U. S. Geological Survey Professional papers and those from other federal and state agencies.

A typical Scarlift-type report contains, first, a description of the watershed, including information such as area, population, land use, geology, and the mining history of the region. Next, the definitions of key terms (i.e., pH, acidity), and the procedures and the results of the watershed study are given. This section describes the general quality and quantity of the water in the basin during the study period. Finally, sections giving the conclusions drawn from the study and recommendations for treatment or abatement measures are included. Most of the reports conclude with several appendices which include all data from the study, various maps of the watershed (i.e., topographic, extent of mining, land use), drawings of recommended treatment measures, and any other appropriate, supporting information.

General Test Site Evaluation. Since there was an extensive amount of literature to search for appropriate test sites, which was impossible for one person to accomplish in a reasonable amount of time, a joint effort was undertaken by five project graduate research associates. The input data needed for the models was categorized into general information topics of physical, climatological, streamflow, deep mine, strip mine, spoil and refuse pile, pyrite reactivity, acid solubility, and cost for treatment. Each topic is further subdivided, but only into general areas. Any possible watershed was to be first rated along these general guidelines, using a scale from 0 to 10, with 0 being unacceptable or totally absent (missing) data and 10 being excellent data available. This is the initial evaluation of possible watersheds; first, allowing elimination of totally unsuitable watersheds due to gross deficiencies of data, and second, indicating a beginning priority of watersheds to study. If only one watershed is being considered, the first evaluation gives an indication of whether to continue with the watershed or to dismiss it as an unsuitable basin. Biemel's Master of Science thesis discusses these evaluations in detail.[4]

Of the 33 mined basin investigations, the use of the general evaluation worksheets indicated that only these eight were worthy of further investigation: Alder Run, Penna.; Beaver Creek, Kty.; Big Scrub Grass Creek, Penna.; Cherry Creek and Casselman River, Md.; Elkins Demonstration Project, W. Va.; Hillman State Park, Penna.; Moraine State Park, Penna.; and Two Lick Creek, Penna.

Detailed Evaluation Worksheets. An intensive study was undertaken next to evaluate the eight chosen watersheds more closely. After a thorough study of the acid mine drainage models, detailed evaluation worksheets were developed which not only account for the nine categories mentioned above, but also for the availability of the data and importance of each data set. Following is a brief discussion of the detailed worksheets used in the evaluation. Biemel's thesis[4] contains an expanded version.

The detailed evaluation worksheets list a certain parameter or an aid in computing that parameter. For example, the watershed area was input to the models and a topographic map aided in determining the area. All the required model input information was listed by category on worksheets. Each parameter (or aid) was assigned an importance factor (IF) ranging from '1', data unnecessary to '4', most necessary. Some examples are: average daily dewpoint temperature '1', total daily solar radiation '2', average ground slope '3', and precipitation data '4'. Next, as a test site was evaluated, a rating from '0', worst, to '10', best, was assigned to each parameter to reflect the goodness of its data. Guidelines were developed to increase consistency, among the different researchers evaluating test sites, for each parameter evaluated. A weighted adequacy number was formed by multiplying its importance factor by its goodness value. These individual weighted parameter values were then tallied as a grade to be assigned to the data group. For example, climatic data might have a score of 34/40. This score can then be used to compare test sites by category data group. This indicates the strength and weakness in certain areas of the reports and permits fairly easy comparison among test sites. These evaluation sheets include reviewer's comments to qualify the data conditions or add other information that might be useful in assembling the data.

A detailed evaluation of a watershed report requires a considerable amount of time. While a reviewer reads the watershed report, he can also complete many sections of the worksheets. However, the report may indicate other sources of data for which the reviewer must search before deciding on the suitability of a particular watershed for modeling.

The detailed evaluation worksheets, being fourteen pages long, were found to be unwieldly for comparing watersheds. The results of these analyses were compiled onto summary sheets to allow easier comparison among several watersheds.

Evaluation of the Data Availability. The previously described analyses were applied to the reports available to this research project. Of the original 33 basins under study, eight were found to contain enough information to merit a detailed study. All of the watersheds were given this analysis, but only the eight indicated earlier were considered for computer modeling. The remaining 25 basins received analyses in an effort to evaluate the detailed worksheets and to provide insight as to data deficiencies. Seven basic topics were analyzed with respect to availability of data and suitability of data included in the reports.

The following chart illustrates the frequencies of occurrence of specific rankings given to several general data divisions required for operating the models. These are based upon about 25 site evaluations. The last column gives a weighted value of the data availability. Generally, scores less than 5 indicate poor status. Following the chart is a discussion of the problems found in the major data categories.

Water Quality Records for the streams are usually available, frequently being monitored at the mine sources or, in some instances, by the USGS in the receiving streams. Groundwater quality records are more frequently not contained in the reports. If they have been considered, they are usually satisfactory. Water quality data is used to check the output from the acid generation portion of the model. Therefore, a '4' would probably result in much difficulty in making an accurate check on the modeling output.

Deep Mine Parameters are determined from mine maps. If maps are not contained within the report, they can sometimes be obtained from the mining companies. Several reports stated that maps were not available for the watershed. Thus, difficulty would arise in assign-

Chart 1.

Categories	Ranking Values											Avg.
	0	1	2	3	4	5	6	7	8	9	10	
Climatological Data	0	0	0	0	0	0	5	10	7	0	0	7.1
Precipitation Data	0	0	0	0	0	0	1	0	6	9	6	8.9
Evapotranspiration	0	0	0	0	2	4	8	5	2	1	0	6.2
Snow Melt Parameters	0	0	0	0	0	4	13	5	0	0	0	6.0
Physical Data	0	0	0	0	3	7	4	4	2	0	0	5.8
Watershed Parameters	0	0	0	0	1	3	6	3	6	2	0	7.1
Interception Parameters	0	0	0	1	4	9	2	1	1	1	1	5.5
Overland Flow	0	0	0	0	0	7	1	3	4	4	2	7.1
Soil Moisture Parameters	1	1	7	3	4	1	2	2	0	0	0	3.4
Streamflow and Routing Parameters	5	3	0	1	1	2	0	5	4	2	0	4.6
Streamflow Parameters	5	1	1	1	2	1	0	1	1	5	2	5.0
Routing Parameters	7	1	1	2	0	7	0	1	2	0	0	3.2
Water Quality Groundwater	0	1	3	5	3	4	1	3	0	0	0	4.1
Quality Parameters	0	1	0	1	1	6	4	3	3	1	0	5.8
Groundwater Parameters	7	5	0	1	6	2	0	2	0	0	0	2.4
Deep Mine Parameters	1	0	1	1	3	3	6	3	1	0	0	5.1
Physical Parameters	1	2	1	1	0	4	2	6	2	0	1	5.4
Complexity of Deep Mine System	0	0	1	1	3	0	2	4	3	3	3	6.9
Acid Removal Parameters	0	2	1	1	2	8	0	3	4	2	0	5.5
Acid Production & Mine Conditions	0	0	1	0	0	12	7	0	0	1	0	5.4
Refuse Pile Inputs	3	0	2	6	3	2	2	2	0	0	0	3.5
Combined Refuse & Pile Strip Mine Model	1	0	4	4	2	3	4	2	0	0	0	4.1
Physical Data	0	0	0	5	6	3	4	1	1	0	0	4.7
Acid Producing Parameters	1	4	2	1	3	7	2	0	0	0	0	3.5

ing values to the parameters. Soil borings and geologic profiles are needed for a portion of the parameters. Most acid production parameters and mine condition parameters will have to be found by trial and adjustment. Since not much information is available on these parameters, their initial values must be estimated. As more information is found or as problems occur in acid mine drainage simulation, these parameters may be adjusted to improve simulation. Due to the lack of mine maps, deep mine parameters are sometimes difficult to obtain. This is often a weak part of the reports. A minimum rank of '5' is acceptable here.

Refuse Pile Parameters. These are usually found by trial. Such data as bulk porosity or pyritic content can be used to determine the acid production rate and solubility of acid product. This information is obtained from pile borings which frequently are missing. A minimum rank of '3' is acceptable because something must be known about the piles in order to make an initial estimate of the parameter values.

Climatological Data is usually obtained from the National Weather Service. When the gaging stations are not in the watershed, particularly in mountainous regions, problems with precipitation records can be substantial. Sometimes watershed precipitation can be synthesized from nearby, outside the basin records. Evaporation data has similar problems plus it may be missing for the winter season at some stations. Of the three subtopics for climatological data (precipitation, evapotranspiration, and snowmelt), precipitation data is usually the most complete,while availability of snowmelt parameters is the most uncertain. The hydrologic model can be run without snowmelt data, but simulation improves with snowmelt. In order to run the model, the overall ranking for climatological data should be at least '5'. This value is frequently attained without much difficulty.

Physical Data Parameters are partially obtained from USGS topographic maps, aerial photographs, and land use maps, which are usually adequately included in the reports. Soil borings, geologic profiles, and well logs needed to assess soil moisture parameters are frequently not included. Watershed parameters and overland flow parameters are the most complete, while soil moisture parameters are the least complete. On the whole, physical data is usually good enough for the models. A value of '5' is the minimum acceptable for physical data.

Streamflow and Routing Parameters are obtained from USGS records and rating curves for the watershed. If a USGS station is not located on the stream, then streamflow data will probably be incomplete. However, having a USGS station does not necessarily guarantee that there will be sufficient data. The frequency chart above shows that in most cases, either streamflow data is satisfactory ('5' or more), or it is totally unacceptable ('0' ranking). Streamflow records are a high-priority data set for the hydrologic simulation portion of the models.

Refuse Pile and Strip Mine Parameter information can be found from borings, topographic maps, and aerial photographs. From the soil borings the coal type can be determined which will be used to determine the pyritic content. This then can be used to find the acid solubility and pyrite reactivity. Some knowledge of the chemistry involved here is desirable. Discussions by Clark et al.[1] will give a good background in this acid chemistry. The parameters for refuse pile and strip mine modeling are often a weak part of the reports. Since many of the values for refuse pile and strip mine parameters must be found by trial and adjustment, a ranking of '4' is required.

Evaluation Conclusions. Many differences occurred in the evaluating and ranking of the modeling parameters for the different watersheds. What one evaluator considered good data on a subject, another considered to be poor data. Even when the evaluators agreed on the quality of the data available, often the ranking values were different. It was therefore necessary to specify the requirements needed for the ranking by compiling a list of definitions for the model parameters and the means and considerations made in each evaluation. These definitions are in Biemel's thesis.[4] Differences, undoubtedly, will continue to exist due to personal biases; however, these definitions should minimize evaluation discrepancies.

The minimum rankings assigned to the various topics are intended to indicate the lowest level at which information pertaining to the particular topic is acceptable for computer modeling. In most cases the rankings should and will be higher than these minimums. Also, if all subtopic rankings are satisfactory except for one, then probably enough work can be done on the unsatisfactory subtopic so that a run can be made.

Throughout the evaluation process, comments concerning where specific pieces of data can be found are necessary. These comments are based on information in the report about what agency collected certain data and where the data is stored. Undoubtedly, all the data needed for both hydrologic and acid mine drainage simulation will not be included in the report, thus these comments serve to remind the researcher where the data can be found. Experience shows that telephone calls and trips to the data holding agency will probably be necessary.

As previously mentioned, eight of the 33 watersheds were deemed worthy of consideration beyond the initial, general evaluation. The evaluations were weighted toward hydrologic and acid mine drainage simulation. If the report of a studied watershed indicated that a particular data set required for hydrologic or acid production simulation was unsuitable or absent, then that report was immediately rejected as having unsuitable data. For example, daily recorded average streamflow is required for hydrologic simulation. In many cases, streamflow measurements were made once per month, or even with less frequency and this lack of acceptable data was cause for immediate rejection of a given basin.

Another area of interest in the watershed review procedure was the amount of reclamation, treatment, or abatement cost information contained in the reports. This information, used in the Basin Optimization Model (another model developed in this research to aid in pollution abatement) for determining optimal acid reduction decisions, must be kept up to date as costs of construction, operation, and maintenance increase. While cost information was not emphasized throughout the reviewing, space for comments on the availability and amount of cost data in each report was provided on the worksheets. This research group found that approximately 75% of the reports contained cost information which the reviewer felt was detailed enough to aid in assessing values for acid controlling measures.

Chosen Study Watersheds. From the evaluation described above, three of the possible eight watersheds appeared most suitable for hydrologic and acid mine drainage simulation. Two of these watersheds are the Roaring Creek basin and the Grassy Run basin near the town of Elkins, West Virginia. These basins border each other and were studied by the U. S. EPA as well as other governmental agencies. The Roaring Creek basin is large (75.63 km^2, 29.2 mi^2) while the Grassy Run basin is comparatively small (7.41 km^2, 2.86 mi^2). The watersheds have the three acid producing mechanisms; that is, strip mines, deep mines, and refuse piles. A complication with these two watersheds is an underground mine that transfers about 12,000 m^3/d (3500 ac-ft/yr) of water from the Roaring Creek basin to the Grassy Run basin.

The third basin chosen is the Cane Branch sub-basin of Beaver Creek in south-central Kentucky. This sub-basin, along with two others on Beaver Creek, were the subjects of an extensive study from 1956 through 1961 under the United States Geological Survey and other state and federal agencies. This is a small sub-basin (1.74 km^2, 0.67 mi^2) containing mainly strip mines and refuse piles with two drift mines.

Intensive effort is now underway on applying the unit source models to these basins. Even those selected as the most promising of the group have major data deficiencies. However, data synthesis techniques are being developed in attempt to salvage these sites for modeling.

SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

Summary. Application of Acid Mine Drainage Unit Source Models requires large amounts of input data. This research group developed and tested a method of systematic watershed evaluation when considering applying these computer models. Many government sponsored mined watershed studies were reviewed using this evaluation procedure and from these reviews an analysis was made of general data deficiencies in the reports. Of the 33 watershed reports reviewed, three were chosen for modeling; Roaring Creek basin and Grassy Run basin near Elkins, West Virginia, and the Cane Branch basin of Beaver Creek, Kentucky.

Conclusions. The major conclusion possible from this study is that the majority of Scarlift-type reports performed on mined watersheds do not result in sufficient collection and publication of data to permit straight-forward hydrologic and acid mine drainage modeling. In general, the reports are strong in water quality data and weak in streamflow data. The models need daily average streamflow as input data, but streamflow measurements were often made no more than twice monthly, far too infrequent for hydrologic modeling. Water quality data, because it is only used for comparing simulated acid loads to recorded acid loads, need not be collected daily, although daily quality data would be ideal.

Daily precipitation and evaporation data are crucial for operating the model. Some of the studies recorded precipitation in the watershed while others did not. Evaporation data was not collected on the site in any case. For accurate simulation using the models, the precipitation data should be collected on the study site, and, if possible, the evaporation should be measured on the site using Class A pans.

A major weakness found in the reports is the lack of usable data for mining parameters; that is, deep mine parameters, refuse pile inputs, and combined refuse pile-strip mine parameters. Information such as void ratio of the strata, minimum flow rate for acid removal by flooding, oxygen concentration in the mines, temperature in the mines, gas diffusivity, acid production rates, solubility of acid products and other parameters are rarely included in coal mine drainage basin reports. Some of these parameters can be evaluated from other data (i.e., pyrite reactivity, soil borings); however, even these ancillary pieces of data are often absent, forcing the reviewer to either search further for the data, go to the watershed and directly collect the data, synthesize or estimate the data, or completely abandon the watershed for acid production simulation.

Recommendations. Six areas of large data deficiencies were found to be common to the majority of mined watershed reports which were reviewed. The first three recommendations given below will aid with the application of the hydrologic model by supplying required input data for adjusting the model to a particular study watershed. The final three recommendations, if followed, are designed to collect the data necessary to run the acid production model and to verify its output. The six recommended steps for data collection are:

(1) Record at least three years of daily streamflow,
(2) Install a recording precipitation gage in the watershed during the period of streamflow gaging,
(3) Install a Class A pan for evaporation in the watershed during the streamflow monitoring period,
(4) Make accurately documented soil borings in spoil piles, and unmined areas within the watershed,
(5) Determine pyrite content of refuse piles and strip mines, and
(6) Record water quality at the watershed outlet and at major acid pollution sources.

The hydrologic portion of the model requires a minimum of three years of daily, average streamflow data in order to self-adjust to conditions of the watersheds. This data is essential, first, to compare simulated streamflow to recorded streamflow for testing the accuracy of simulated flow, and secondly, to internally adjust certain parameters to improve streamflow simulation when a comparison of simulated and recorded streamflow indicates unacceptable differences between them. Thus, daily streamflow gaging is recommended for any future watershed monitoring projects.

Due to the dependence of the hydrologic model on large quantities of input data, and because the accuracy of this data is of utmost importance, a recording, year-round precipitation gage in the watershed is of prime importance. This gage, when properly maintained and used for the entire stream monitoring period, will provide an accurate account of all water entering the basin as precipitation, thereby removing the problems of heavy localized rainfall at a precipitation gage outside the watershed while the watershed receives no precipitation, or vice versa.

Class A pan evaporation data, another essential data group, should be collected on the watershed throughout the duration of streamflow gaging. Daily, year-round evaporation data on the watershed removes the need to search for suitable nearby evaporation data stations and it assures that the evaporation data is representative of that in the watershed.

Accurately documented soil borings are important so as to assure precise description of certain hydrologic inputs as well as to aid in determining acid production parameters. These borings should record the types of soil encountered, the depths to and thicknesses of the different soil types, the level at which groundwater is reached, and also other data, such as permeability, porosity, or void ratio, which will assist in establishing input parameters.

Pyrite content of refuse piles and strip mines provides the means of determining several acid-production-related parameters. Actual on-site pyritic content data, as opposed to estimated values made in the absence of field data, gives the most accurate acid mine drainage simulation, thus making collection of pyritic content data important.

Finally, a record of the quantity and quality of acid mine discharge from major acid pollution sources into the receiving stream is of value for comparing the simulated acid loads with actual field data. The deep mine discharges, while not subject to the large fluctuations encountered with surface phenomena, do have long-term variations which the computer simulation must reflect. The quantity and quality of strip mine and refuse pile drainage varies much more quickly than that of deep mines because strip mine and refuse pile drainage depends largely on surface runoff, a response occurring during and immediately after precipitation. The water quantity and quality from major acid production sources, as well as the water quality at the basin outlet, should be monitored at a minimum of once every second week, more frequently when feasible. Several times during the period of data collection, the quantity and quality of runoff from strip mines and refuse piles should be monitored immediately following precipitation in order to check the simulated values against the actual data.

In closing, it may be said that any good mine drainage models (present or future) for acid mine drainage are going to need the aforementioned types of data to verify and calibrate them. Therefore, it is highly recommended that future demonstration projects or monitoring endeavors have their data collection schemes consider the parameters discussed herein before the data collection gets too far along to permit the proper acquisition of the crucial pieces.

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A MODELING TECHNIQUE FOR OPEN DUMP BURNING

Marvin Rosenstein
Systems Analysis Branch
U.S. Environmental Protection Agency (EPA)
Region I, Boston, Massachusetts

Valentine J. Descamps
Regional Meteorologist*
U.S. Environmental Protection Agency (EPA)
Region I, Boston, Massachusetts

ABSTRACT

This paper describes a modeling technique for estimating the impact of open dump burning upon ambient particulate concentrations. The technique is based upon two major assumptions. First, the entire area of the dump is not fired at the same time. Rather, it is assumed that the dump burns "progressively" with a constant rate at which the fire spreads through the dump. Second, once a portion of the dump is fired, the total burn time for that portion consists of an initial "hot phase" followed by a longer "smolder phase". Plume rise is based upon Briggs' formulations and diffusion calculations are performed by the EPA point source model PTDIS. The technique is crude and no attempt has been made to validate it with field data. Limitations of the technique and suggestions for improving it are discussed.

BACKGROUND

Primarily for economic reasons, several New England states are permitting towns, particularly small rural communities, to use open dump burning for the disposal of community solid waste under variance procedures until more environmentally acceptable disposal methods are implemented. Because of their concern for the maintenance of adequate air quality, the Department of Environmental Protection of the State of Maine requested assistance from us in developing a technique for estimating the impact of open dump burning upon ambient particulate levels. (Note that EPA regards open dump burning as hazardous to air quality, public health, and water quality and opposes it as a permanent solution to the disposal of solid waste.) Discussion with other EPA personnel in the fields of diffusion modeling and solid waste disposal, as well as a literature search, revealed scant information upon which we could base the development of a technique. Also, the press of operational duties, which leave little time for development activities, dictated that the technique should utilize existing diffusion and plume rise formulations that could be rapidly and conveniently applied. It was therefore recognized at the outset that the technique would of necessity be crude and most likely conservative in nature, such that predicted concentrations could be regarded as upper bounds.

THE NON-PROGRESSIVE TECHNIQUE

Our first attempt at a modeling technique involved what we call a "non-progressive" burn. Although we later discarded this technique, we will describe it in some detail because many of the features and assumptions of this technique carry over to our final "progressive" model. Also, we feel that the idea of a progressive burn is of paramount importance and can only be fully appreciated when viewed against the background of a non-progressive burn.

In the non-progressive approach, we assume that the entire area of the dump is set on fire at the same time. Gerstle and Kemnitz[1], based on laboratory simulations of the open burning of municipal refuse, suggest a total burn time of 12 hours consisting of an initial "hot phase" of duration 1 to 1½ hours followed by a "smolder phase" for the remainder of the 12 hours. (In future sections, subscript A will always refer to the hot phase and subscript B will always refer to the smolder phase). Approximately 90% of the refuse burns rapidly during the hot phase, and the remainder burns slowly during the smolder phase. After consultation with regional personnel in the field of solid waste disposal (hereafter referred to as regional personnel) we settled on a (1 hour - 75%) hot phase and an (11 hour - 25%) smolder phase. We assumed that the refuse burns fairly evenly with respect to time during each of the two phases. Gerstle and Kemnitz also suggest an emission factor of 16 pounds of particulates per ton of refuse burned. The State of Maine suggested that each person generates 20 pounds of refuse per week. With these figures one can easily calculate particulate emission rates for the first hour and for each of the next eleven hours. Populations of 1000, 2000 and 3000 were considered.

The hourly concentrations for each of the twelve hours were calculated as follows. First, plume rise was calculated using Briggs' (2,3,4) formulations. The buoyancy flux, F, was calculated via the equation below.

$$F(m^4sec^{-3}) = KQ_H, \quad K = (3.7)\cdot(10^{-5})m^4cal^{-1}sec^{-2} \tag{1}$$

The heat emission rate Q_H(cal sec^{-1}) was easily calculated for each of the twelve hours from the computed pounds of refuse burned per hour and the heat factor of 4675 Btu per pound of refuse burned. This heat factor was extracted from Lowe[5] who states that it is for municipal waste that has had some separation treatment for use in a power boiler. A lower value seems more appropriate to unsegregated residential/commercial waste that may be dampened by exposure to a generally moist climate. After consultation with regional personnel we decided to run the technique for an additional case that used a heat factor of 2000 Btu.

Diffusion calculations, using the emission rates and plume rises as determined above, were performed by the EPA point source model PTDIS developed by Turner[6] and based on the steady-state Gaussian formulations as detailed in Turner[7]. This model computes hourly centerline concentrations at specified (by the user) distances downwind of an isolated point source in relatively flat and open terrain and for a rural atmosphere. Meteorological conditions consisting of stability class, wind speed and mixing height are input by the user. We used seven receptor distances from 0.1 to 10.0 km and four meteorological conditons of stability classes B and F combined with wind speeds of 1.0 and 5.0 m sec^{-1}. Constraints on vertical dispersion via a mixing height were not included. For each combination of meteorology, population and heat factor only two diffusion calculations are necessary, i.e., one for the hot burn hour that yields an hourly concentration of X_A and one for the smolder burn type

*On assignment from ARL/NOAA Department of Commerce of hour that yields an hourly concentration of X_B (the same value for each of the eleven smolder hours). The 24-hour concentration is therefore calculated through the relationship presented below.

$$\bar{X} = \frac{X_A + 11X_B}{24} \qquad (2)$$

Before presenting some results for the non-progressive technique, several conservative assumptions should be pointed out since they will also apply to the progressive model developed in the next section. First, a given stability-wind speed condition persists for the entire burn time. Second, only centerline concentrations are calculated. Therefore, a constant wind direction over the entire burn time is assumed. Third, the dimensions of the dump are small enough such that the dump can be considered a point source instead of an area source. A line source model was considered for the technique but was discarded after trial calculations which invoked assumptions concerning the dimensions of the dump produced results essentially identical to those obtained with the point source model.

Tables 1 and 2 present some results for the non-progressive technique for the wind speed of 1.0 m sec^{-1}. The effect of reducing the heat factor from 4675 Btu to 2000 Btu is dramatic with maximum concentrations increased by a factor of two or more due to the smaller plume rises. For the 5.0 m sec^{-1}case, the overall maximum concentrations were 47 and 93 ug m^{-3} for the 4675 and 2000 Btu heat factors respectively. The large increase in maximum concentration from the 1.0 m sec^{-1}case to the 5.0 m sec^{-1}case indicates the dominance of the effect of wind speed on plume rise over that of the wind speed on dilution. There is some tendency for maximum concentration to increase with increasing population (particularly for the 5.0 m sec^{-1} case which is not shown) although this is not always the case because of the competing effects of increasing emissions versus increasing plume rises.

Table 1

Final Plume Rise (m) during (hot phase/smolder phase) for non-progressive technique and wind speed of 1.0 m sec^{-1}

Population	1000	2000	3000
Stability B			
4675 Btu	896/78	1359/131	1735/178
2000 Btu	528/41	799/68	1020/93
Stability F			
4675 Btu	129/40	162/50	185/58
2000 Btu	97/30	122/38	140/44

Table 2

Maximum 24-Hour Concentrations (ug m^{-3}) for non-progressive techniques and wind speed of 1.0 m sec^{-1}

Population	1000	2000	3000
Stability B			
4675 Btu	5	4	3
2000 Btu	11	13	9
Stability F			
4675 Btu	9	9	10
2000 Btu	17	21	21

THE PROGRESSIVE TECHNIQUE

Discussion of the non-progressive technique with the State of Maine and regional personnel indicated several improvements could be made. Particularly alarming were some of the very large plume rises as given in Table 1. Field observations by Maine indicated that such large plume rises do not occur. These same field observations also indicated that the total burn time is more likely to be on the order of twenty-four hours and that an entire dump is not normally fired at once. Instead, the fire normally spreads through the dump at a gradual rate such that it takes hours for the entire dump to be fired. This consideration lead to the development of the progressive model.

In the progressive technique, it is assumed that the dump is fired progressively at a constant rate (which can be varied from case to case) such that the fire gradually spreads through the dump. The rate of spreading should depend on prevailing meteorological conditions but this effect is ignored in the cases to follow. Once a portion of the dump has been fired, the assumption of a hot phase-smolder phase regime applies in the same way as for the non-progressive technique. As an example, refer to Table 3. Here we have assumed a total burn time of twelve hours. In the first hour, 1/6 of the dump is fired and part of this portion of the dump is consumed in a hot phase burn. The remaining part of this portion of the dump smolders over the following six hours (hours 2 through 7). In the second hour, another 1/6 of the dump is fired. The smolder phase now lasts for hours 3 through 8. And on it goes. It takes a total of six hours for the entire dump to be fired. Each block in Table 3 gives the partial contributions of each 1/6 portion of the dump to the total hourly concentrations listed at the bottom of the table. As with the non-progressive technique, only two basic diffusion calculations need to be done. In contrast to equation (2) for the non-progressive twelve hour burn, the 24-hour average concentration is calculated via the equation below.

$$\bar{X} = \frac{6X_A+(6)(6)X_B}{24} = \frac{X_A+6X_B}{4} \qquad (3)$$

The technique can be generalized (for total burn times of 24 hours or less) as follows. Let Y equal the number of hours it takes for the fire to spread through the entire dump, i.e., 1/Y of the dump is fired in each of the first Y hours. Let S equal the number of hours that each 1/Y portion of the dump smolders. Then the 24-hour average concentration is calculated by the equation below.

$$\bar{X} = \frac{\sum_1 X_i}{24} = \frac{(Y)X_A+(Y)(S)X_B}{24} \qquad (4)$$

Therefore, for a 24-hour burn with a hot phase duration of 12 hours, and a 12 hour smolder duration, we have

$$\bar{X} = \frac{12X_A+(12)(12)X_B}{24} = \frac{X_A+12X_B}{2} \qquad (5)$$

The progressive technique can also be used for total burn times of greater than 24 hours, but the general relationship expressed in equation (4) will not hold. But equations similar to equations (3) and (5) can still be derived from tables constructed like Table 3.

Table 3

Twelve Hour Progessive Burn Sequence, Hot Phase Duration = 6 hours, Smolder Phase Duration = 6 hours. See discussion in text for explanation.

HOUR	1	2	3	4	5	6	7	8	9	10	11	12
HOT BURN	X_A	X_A	X_A	X_A	X_A	X_A						
SLOW BURN DUE TO FIRE IN HOUR #												
1		X_B	X_B	X_B	X_B	X_B	X_B					
2			X_B	X_B	X_B	X_B	X_B	X_B				
3				X_B	X_B	X_B	X_B	X_B	X_B			
4					X_B	X_B	X_B	X_B	X_B	X_B		
5						X_B	X_B	X_B	X_B	X_B	X_B	
6							X_B	X_B	X_B	X_B	X_B	X_B
TOTAL HOURLY CONCENTRATIONS X_i, $i=1, 12$	X_A	X_A + X_B	X_A + $2X_B$	X_A + $3X_B$	X_A + $4X_B$	X_A + $5X_B$	$6X_B$	$5X_B$	$4X_B$	$3X_B$	$2X_B$	X_B

The particulate and heat emission rates, Q_P and Q_H that are required for the diffusion and plume rise calculations can be calculated from the following equations:

$$Q_{PA} = .75\frac{(E_p)}{Y} \qquad Q_{PB} = .25\left(\frac{E_p}{(Y)(S)}\right) \qquad (6)$$

$$Q_{HA} = .75\frac{(E_H)}{Y} \qquad Q_{HB} = .25\left(\frac{E_H}{(Y)(S)}\right) \qquad (7)$$

$$E_p = (\text{population}) \left(\frac{\text{lbs refuse}}{\text{person}}\right) \left(\frac{\text{lbs particulates}}{\text{pound of refuse}}\right) \qquad (8)$$

$$E_H = (\text{population}) \left(\frac{\text{lbs refuse}}{\text{person}}\right) \left(\frac{\text{Btu}}{\text{pounds of refuse}}\right) \qquad (9)$$

The plume rise calculations and diffusion calculations are performed in the same way that they were for the non-progressive technique. The same conservative assumptions that were discussed in the section on the technique apply here as well. Each portion of the dump that is fired is considered a point source and separation distances between the various portions are ignored. Meteorology is constant for the duration of the burn.

Three cases using the progressive technique were investigated. Table 4 lists the assumed values for the operating parameters for each case. Equation (3) applies in case 1, while equation (5) applies in cases 2 and 3. Receptor distances of 0.1, 0.25, 0.4.0.7,1.0, 1.5, 2.0, 2.5 and 3.0 km were used. A representative range of up to 22 stability-wind speed combinations were investigated.

Table 5 lists some of the calculated plume rises for the three cases for a wind speed of 1.0 m sec^{-1}. Table 5 is constructed in the same fashion as Table 1 to enhance comparisons between the non-progressive and progressive techniques. The plume rises are purposely listed for the 1.0 m sec^{-1} case for two reasons. First, the inverse relationship between plume rise and wind speed implies that the listed plume rises should be representative of the maximum rises that can be expected. Second, high wind speeds are not relevant because of the danger of spreading fire to areas surrounding the dump. The progressive cases yield plume rises that are much less than those of the non-progressive cases. The most realistic plume rises appear to be those for progressive case number 2 which yields plume rises generally less than 200 m.

Table 5

Final Plume Rise (m) during (hot phase/smolder phase) for progressive technique and wind speed of 1.0m sec^{-1}

Population	1000	2000	3000
Stabilities (A-D)			
Case 1	223/26	374/43	487/58
Case 2	87/6	146/10	198/14
Case 3	164/11	277/19	375/26
Stability E			
Case 1	78/30	98/37	112/43
Case 2	51/16	64/20	74/22
Case 3	68/21	86/26	98/30

Table 6 presents a selection of predicted 24-hour concentrations under neutral (D) stability and wind speeds of 1.0 and 5.0 m sec^{-1} for the three progressive cases. Results for these meteorological conditions were chosen for presentation because of the prevalence of these meteorological conditions in many sections of New England and because only neutral stability can persist for 24 hours. Neutral stability also generally yielded the highest predicted concentrations. As previously discussed, observations in the field by the State of Maine personnel indicate cases 2 and 3 to have the most realistic operating parameter. It is for these cases that the technique indicates a potentially serious threat to the National Ambient Air Quality Standards of 260 ug m^{-3} (primary) and 150 ug m^{-3} (secondary) for 24-hour average concentrations of particulates. Case 2 yields the most realistic estimates of plume rise and the highest predicted concentrations.

DISCUSSION OF PROGRESSIVE TECHNIQUE

Thus far, we have not been able to obtain sufficient data with which we could attempt to validate the technique. However, it is encouraging that the technique is able to produce plume heights that seem

Table 4

Assumed Operating Parameters for Three Progressive Burns

	Total Burn Time (Hours)	Hot Phase Duration (hrs)	Smoulder Phase Duration (hrs)	Heating Value Per lb waste (Btu/lb)	Waste Per Person (lbs/person/week)	Emission Factor lbs of particulate per ton of waste(lbs/T)
Case 1	12	6	6	3500	20	16
Case 2	24	12	12	2000	20	16
Case 3	24	12	12	4675	20	16

Table 6

Predicted 24-Hour Average Concentrations (ug m^{-3}) for progressive techniques, neutral (D) stability, wind speeds of 1.0 and 5.0 m sec^{-1}, (X = concentration less than State of Maine Standard of 100 ug m^{-3}).

Town Size in Population Count

	Wind Speed m/sec	1000					2000					3000				
		Distance Km														
		0.1	0.25	0.4	0.7	1.0	0.1	0.25	0.4	0.7	1.0	0.1	0.25	0.4	0.7	1.0
Case 1	1	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	5	192	X	X	X	X	128	X	X	X	X	X	108	X	X	X
Case 2	1	786	288	138	X	X	348	426	240	102	X	X	432	300	144	X
	5	366	115	X	X	X	647	139	X	X	X	889	201	100	X	X
Case 3	1	X	186	114	X	X	X	132	138	X	X	X	X	108	X	X
	5	313	X	X	X	X	504	127	X	X	X	576	180	X	X	X

reasonable on the basis of rural sightings of dump plumes. As for predicted concentrations, without sufficient field data to compare them with, about all we can say is that they do not seem implausible.

The technique has two important advantages. First, it is relatively easy to use, being based upon familiar and readily available diffusion and plume rise formulations. Secondly, the technique can be easily tuned via the values that must be assumed for the following operating parameters: total burning time, hot phase duration, smolder phase duration, fraction of refuse consumed in each phase (values other than 75% for the hot phase and 25% for the smolder phase may be appropriate), pounds of refuse generated per person, pounds of particulates generated per ton of refuse, and the heating factor (Btu per pound of refuse).

As previously discussed, the technique as it presently exists has several limitations that may introduce a very high degree of conservatism into the predictions. The very bad assumption of constant meteorology as well as the lesser evil of using point sources instead of areas sources could both be remedied through suitable computer programming. The virtual point source concept could be introduced to handle area source configurations. The technique could also be changed so as to allow meteorological input (stability, wind speed and wind direction) that varies from hour to hour and receptor locations that vary in both horizontal directions. Unfortunately, as discussed in the background section, we did not, nor are we likely to ever, have the time to carry out the above suggestions.

In conclusion, we believe that we have developed a technique that is potentially very useful for estimating the impact of open dump burning upon ambient particulate levels. Furthermore, we believe it is worthy of future efforts to both improve it and establish its validity.

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DEVELOPMENT AND USE OF A FIXED CHARGE PROGRAMMING MODEL FOR REGIONAL SOLID WASTE PLANNING*

Warren Walker
The New York City-Rand Institute

Michael Aquilina
Champlin Petroleum Company

Dennis Schur
U.S. Environmental Protection Agency

Abstract

The problem of deciding on the number, type, size and location of the solid waste disposal facilities to operate in a region, and allocating the region's wastes to these facilities is formulated as a fixed charge problem. A system for solving this problem, developed for the U.S. Environmental Protection Agency is described. The system includes a heuristic algorithm for the fixed charge problem. A description is given of a hypothetical application of the system in the Seattle-King County region of the State of Washington.

Introduction

Solid waste management is a crucial problem facing every municipality. The average person generates over five pounds of material per day for which he no longer has any use and, therefore, discards. Among the services supplied by most municipal governments is the collection, transport, and disposal of such solid wastes.

The collection operation consists of the removal of solid waste (usually in a truck) from its point of generation. It is then transported to an intermediate facility or an ultimate disposal site. At an intermediate facility it may undergo some processing (such as incineration, resource recovery, biochemical oxidation, or compaction) that leaves a residue of waste that must still be disposed. Most ultimate disposal sites are sanitary landfills.

Prior to their explosive growth in the 1950's and 1960's, most cities had no problem disposing of all their solid waste within their own borders. However, as available land begins to disappear and sites begin to be used up, cities are beginning to look outside their own boundaries for disposal sites. In addition technological processes for waste reduction and recycling are too expensive and inefficient for single municipalities to consider using. But, by taking advantage of economies of scale, such facilities can be built and operated for use by several municipalities with a net cost saving to the region as a whole.

Therefore, an increasing number of cities, towns, and villages are joining together to perform solid waste planning for an entire region. For example, in New York State, 35 percent of the State's 1500 municipalities use solid waste disposal facilities operated in cooperation with other units of local government.

Several recent studies have dealt with the minimization of transportation and disposal costs in regional solid waste management systems. Anderson[2] developed an algorithm for determining the optimum solution to a regional disposal problem, but his model assumes that all costs are linear.* Marks and Liebman[5] treat the more limited problem of determining the locations of transfer stations and include the fixed costs of building and operating such facilities in their formulation.** The special structure of the resulting problem (a capacitated transshipment problem) allows them to obtain optimal solutions using a minimum cost--maximum flow network algorithm.

In[6], Morse and Roth formulate the problem without capacity constraints and attempt to solve it by complete enumeration, comparing the costs resulting from each of the 2^j-1 solutions for a given set of j possible disposal facility locations. Kuhner and Harrington solve a similar problem using the branch-and-bound algorithm that is part of IBM's MPSX-MIP program[4].

The formulation that Skelly developed[8] provides the basis for the model described in this paper. To solve his problem he used an early version of the computer program we describe.

In this paper we develop an integer programming model for selecting from potential and existing sites those that should be developed, at what capacity and how the wastes should be routed through them so that the total transport, processing, and disposal costs for the entire region are minimized. Fixed charge cost functions are included for all facilities, as is a consideration of the time-staging of the construction of facilities.

The output from the model provides information on:

- What types of disposal facilities should be built?
- When should they be built?
- What should be their capacity?
- How much of its solid waste should each community ship to each of the disposal facilities?
- What will be the cost of the solution (both fixed cost and cost per ton)?

It is what Marks and Liebman[5] refer to as a capacitated transshipment facility location problem, with fixed and variable costs associated with the use of each facility and variable haul costs. A heuristic algorithm has been developed that produces solutions that are almost always optimal. This algorithm has been embedded in a computer program that includes a routine for generating the problem matrix and a report generator for displaying the results. The program has been given the name "SWAM" for Solid Waste Allocation Model.

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* Figures in superscript refer to bibliographical references listed at the end of this paper.

** Transfer stations are intermediate facilities where collection vehicles transfer their loads to larger vehicles, more suited for long-haul transportation. The larger vehicles transport the waste to the disposal site.

In the following sections we describe the mathematical model, the heuristic algorithms used to solve it, and the data requirements of the SWAM model. A sample application of the SWAM model using data from the Seattle region where the model was used in a regional planning effort during 1973 will be presented at the Conference but cannot be included with the text of this paper due to the excessive space requirements.

The Mathematical Model

In order to simplify the problem and make it computationally feasible to solve, we assume that all the refuse of a community is generated at a single point, its center of mass, and, therefore, that all waste transported from the community travels from its center of mass. This permits us to separate the transport and disposal subsystems from the collection subsystem.

We assume that there are K potential disposal sites being considered, J intermediate facilities, K-J final disposal sites, and that there are N communities.

The general problem formulation for the one-period (say, one week) static model is:

$$\text{Minimize} \quad \sum_{k=1}^{K} \sum_{i=1}^{N} C_{ik} x_{ik} + \sum_{k=j+1}^{K} \sum_{j=1}^{J} C_{jk} x_{jk} + \sum_{k=1}^{K} F_k \delta_k$$

Subject to

$$\sum_{k=1}^{K} x_{ik} = W_i \quad (i=1,2\ldots,N)$$

$$\sum_{i=1}^{N} x_{ij} \leq A_j \quad (j=1,2,\ldots,J)$$

$$\sum_{i=1}^{N} x_{ik} + \sum_{j=1}^{J} x_{jk} \leq B_k \quad (k=J+1,\ldots,K$$

$$P_j \sum_{i=1}^{N} x_{ij} - \sum_{k=J+1}^{K} x_{jk} = 0 \quad (j=1,\ldots,J)$$

$$\sum_{i=1}^{N} x_{ij} - y_j = 0 \quad (j=1,\ldots,J)$$

$$\sum_{i=1}^{N} x_{ik} + \sum_{j=1}^{J} x_{jk} - y_k = 0 \quad (k=J+1,\ldots,K)$$

$$\delta_k = \begin{matrix} 0 \text{ if } y_k = 0 \\ 1 \text{ if } y_k > 0 \end{matrix} \quad (k=1,2\ldots,K)$$

$$x_{ik} \geq 0 \quad (i=1,2,\ldots,K)$$

$$y_k \geq 0 \quad (k=1,2,\ldots,K)$$

where:

C_{ik} is the cost of transporting and processing one ton of waste from source i at disposal facility k ($/ton);

C_{jk} is the cost of transporting and processing one ton of waste from intermediate facility j at final facility k ($/ton);

F_k is the fixed cost associated with opening and operating disposal facility K ($/week);

W_i is the quantity of waste generated at source i (tons/week);

A_j is the capacity of intermediate site j (tons/week);

B_k is the weekly capacity of final disposal site k (B_k depends upon the number of trucks the site can handle, and, since landfill sites get filled up, the length of time it is desired to operate the site) and;

P_j is the proportion of the weight of the waste that remains after being processed at intermediate site j.

The decision variables are:

x_{ik} (i=1,2,...,N; k=1,2,...,K): the amount of community i's waste that is to be sent to disposal facility k; and

x_{jk} (j=1,2,...,J; k=J+1,...,K): the amount of waste that is to be transported from intermediate disposal facility j to final disposal facility k.

The Constraints

We discuss each of the constraining equations in turn.

- Constraint (2.2) requires that all of the solid waste generated at a source during one week be transported to some disposal facility during the same week.
- Constraint (2.3) recognizes the limited processing capacities of incinerators and transfer stations. If this constraint is omitted, the model can be used to determine a desirable capacity for a proposed facility.
- Constraint (2.4) recognizes the limited capacity of a landfill site. Its weekly capacity depends on its ultimate capacity (say, T tons) and its targeted useful life (say, Y_k years).[k] Then B_k is given by: $B_k=T_k/52\ Y_k$. The weekly capacity may also be affected by the capacity of access roads to handle traffic without congestion, and the unloading rate at the landfill site.

- Constraint (2.5) is a balance equation for intermediate sites. It specifies that whatever waste is received at an intermediate site must be shipped from that site to a final disposal site, adjusted for the weight reduction produced by intermediate processing.

- Constraints (2.6), (2.7), and (2.8) insure that the fixed costs of building and operating a disposal facility are included in the objective function if the site is to be utilized at a positive level. If site k is utilized, y will be greater than zero and δ will assume the value "1". Thus, the fixed cost F_k associated with facility k would be added to the value of the objective function. If site k is not utilized y_k will be zero, δ will be zero, and F_k will not be added to the objective function.

- Constraints (2.9) and (2.10) are the non-negativity constraints on the x_{ik}'s and y_k's.

The Objective Function

The objective of this model is the minimization of the total regional costs of solid waste disposal. These costs include transport costs (from a community to an intermediate site, from a community to a landfill site, and from an intermediate site to a landfill site), and operating and capital costs associated with a disposal facility.

We assume that each of the individual components of total cost can be represented by one of the two types of cost functions shown in Figs. 1 and 2.

Typically, the cost of transporting waste from a site i to site k can be represented by a linear function (Fig. 1) of the amount of waste shipped. We will let H_{ik} be the unit transportation cost.

The cost function associated with each disposal facility, k, is of the form shown in Fig. 2. There is a fixed initial construction and/or overhead cost, F_k, as well as variable operating costs, V_k, which are dependent on the amount of waste processed.

Each cost factor C_{ik} or C_{jk}, defined above, is therefore, the sum of a unit transportation cost and a unit operating cost. That is:

$$C_{ik} = V_k + H_{ik} \qquad (i=1,2,\ldots,N; K=1,2,\ldots,K)$$

$$C_{jk} = V_k + H_{jk} \qquad (j=1,2,\ldots,J; k=j+1,\ldots,K).$$

In many cases the operating cost curves for facilities such as incinerators and transfer stations are not linear, but exhibit economics of scale. We will assume that any such curve can be represented by a piece-wise linear concave cost function such as that shown in Fig. 3. In this illustration there are three different operating ranges. If less than h_2 tons are shipped to the facility, the operating cost is c_1 dollars per ton; for between h_2 and h_3 tons, it is c_2 dollars per ton; and for above h_3 tons, it is c_3 dollars per ton. The three segments of the cost curve, when extended, intercept the y-axis at points f_1, f_2, and f_3.

Such a function can be easily represented as a fixed charge cost function and added to the general objective function derived above. For the example shown in Fig. 3, define new decision variables $\Delta 1$, $\Delta 2$, and $\Delta 3$, corresponding to the three segments of the cost curve (in general, the curve can have any number of segments). With each Δj, associate the variable cost c_j and the fixed cost f_j, so that the cost function for each Δ_j is of the form shown in Fig. 2. Then the general formulation is modified as follows:

- One constraint is added to the problem:

$$x - \sum_j \Delta_j = 0$$

- The following terms are added to the objective function:

$$\sum_j [c_j \Delta_j + f_j \delta_j]$$

- A fixed charge constraint is added for each variable:

$$\delta_j = \begin{matrix} 0 \text{ if } \Delta_j = 0 \\ 1 \text{ if } \Delta_j > 0. \end{matrix}$$

Note that no upper or lower bound constraints need be put on the Δ_j's. It is shown in [9] that, if Δ_j is positive in an optimal solution to the problem

(1) all other Δ associated with that cost function will be zero, and

(2) $h_j \leq \Delta_j \leq h_{j+1}$.

Non-Linear Facility Costs

Of course, not all facility costs will be linear or piece-wise linear. In the case of a non-linear concave cost curve, a piece-wise linear cost function is used as an approximation, as shown in Fig. 4. In order to properly approximate such non-linear functions, the model breaks the cost curve into segments and performs a linear least-squares regression on each segment of the curve.

For example, the best linear fit for the first segment of the function $y=f(x)$, shown in Fig. 4, is determined as follows: Let the required linear approximation be $y=c_1x + f_1$, where c_1 and f_1 are to be determined. The error between the linear approximation and the actual function at any point x is given by:

$$E = f_1 + c_1x - f(x).$$

The square of the error is given by:

$$ES = (f_1 + c_1x - f(x))^2,$$

and the sum of these squared errors is:

$$SSE = \int_{h_1}^{h_2} (f_1 + c_1x - f(x))^2 dx,$$

where h_1 and h_2 define the region of fit.

The minimization of the sum of the squared errors is accomplished by setting the partial derivitives of SSE equal to zero. That is,

$$\frac{\partial SSE}{\partial f_1} = 0, \text{ and}$$

$$\frac{\partial SSE}{\partial c_1} = 0.$$

This produces two equations in two unknowns that can be solved by simple substitution. The solution of this set of equations provides the slope, c_1, and intercept f_1, for the best straight line approximation of the function $f(x)$ between h_1 and h_2. This same procedure is followed for each of the segments of the non-linear cost curve.

Multi-Year Planning Considerations

The mathematical model described above assumes that every week or year in the planning period looks the same as every other week or year (in terms of costs and waste production) and that any site selected is available at the start of the planning period and lasts for the entire period. The optimization of this system is a gross simplification of real-world problems.

In the Solid Waste Allocation Model,the concept of "staging," breaking the planning period into several smaller periods, is used to provide a more realistic solution. One fixed charge problem is solved for each period. Although each period is solved separately and independently from all other periods, remaining ultimate capacities of facilities such as landfills are transferred and updated from stage to stage. At the end of the planning period the results for each of the stages are summarized and totaled to determine the overall cost for the planning period. The number and duration of the periods are determined partly by the user and partly by the program. The closing of a facility, the opening of a new facility, and the creation of a new waste source will all cause a new stage to be started (i.e., a new problem to be solved). The user supplies all opening and closing dates as well as ultimate capacities. In addition, if a facility reaches its ultimate capacity during one of these user-defined stages, the program will create a new stage, and a fixed charge problem with this facility eliminated will be solved to determine where the waste that had been going to that facility should now be transported.

Although there is no real interdependency between stages, the concept of "staging" does allow for a great deal of flexibility in creating a realistic solid waste plan.

The Solid Waste Allocation Model

The Solid Waste Allocation Model (SWAM) is a system of FORTRAN programs that has been developed by the U.S. Environmental Protection Agency's Office of Solid Waste Management Programs under contract to Roy F. Weston, Inc.[1,3] to solve the fixed charge integer program (2.1)-(2.10). It accepts as input some simple data on the disposal facilities and the communities in the region under consideration, and calculates the coefficients for the integer program. It then solves the problem for one or more stages, and prints output reports summarizing the solution.

The following sections briefly discuss the model's data requirements and the heuristic algorithm used in the solution of the problem. The output reports are described as part of the discussion of the application of the model to be covered in the verbal presentation of this paper.

Data Requirements

In order to properly model the transportation, processing, and disposal components of solid waste planning, some specific and detailed data are required. These data are divided into three categories: (1) source data; (2) facility data; and (3) transportation data.

The "source" in SWAM is a point of waste generation that represents a reasonably large residential area, such as a census tract, transportation zone, or planning district. The quantities of waste generated at these sources, specified in tons per week, will be allocated by the model to various processing and disposal facilities. Associated with each waste source, in addition to the generated waste, is a haul cost (in dollars per ton-hour). This cost is used to convert the transportation time from the source to each facility into a dollar cost. The haul cost is a function of the collection vehicles and crews associated with the specific source.

The Solid Waste Allocation Model considers both intermediate and ultimate disposal facilities. The basic data necessary to define an intermediate facility are the maximum operating capacity in terms of tons per week, an operating cost curve, the capital cost of the facility, associated useful life, and the transfer coefficient indicating the percentage weight of incoming waste that will remain after processing. In addition, a unit haul cost (in dollars per ton-hour) is required in order to convert the transportation times from intermediate facilities to ultimate disposal sites into dollar costs. To define an ultimate disposal site the following pieces of data are needed: the maximum operating capacity in tons per week, the ultimate capacity in tons, the capital cost of the facility, an operating cost curve, and a useful life. The operating cost curve associated with a disposal facility can be one of three types: (1) straight line of the form y=ax+b; (2) semi-log of the form log y=ax+b; and (3) log-log of the form y=a log x+b. Curve types (2) and (3) are approximated by piece-wise linear curves using the linear regression procedure described in Section II.

In order to determine allocations of waste from sources to facilities, the model must be supplied with the set of paths along which the waste can be transported. These paths are defined by pairs of locations which can indicate paths from sources to intermediate facilities, from sources to ultimate disposal sites, or from intermediate facilities to ultimate sites. The transportation time in minutes plus the turnaround time at the facility must be supplied for each pair of locations.

The data described above are all that is necessary to run the model for one time period. There are other options in the model, such as multi-year planning and automatic path generation, each with its own data requirements, which will not be described here.

Solving the Fixed Charge Problem

The problem formulated in Section II is a fixed charge problem, which is a special type of integer programming algorithm. It can be solved exactly by any mixed integer programming algorithm. Unfortunately, these algorithms are generally too slow to solve the large problems constructed for practical applications in a reasonable amount of time (although Kuhner and Harrington report some success using IMB's MPSX-MIP system on large problems[4]).

The United States Environmental Protection Agency's Office of Solid Waste Management Programs, therefore, decided to use a heuristic algorithm developed by Warren Walker to solve the problem. The algorithm is described completely in [9], where its speed of execution and optimality of solutions are compared to other solution techniques. It was found to be computationally efficient and sucessful in producing the optimum solution a high percentage of the time.

The algorithm consists of two phases. The first phase is identical to the standard simplex method of linear programming, except that the method of choosing the vector to bring into the basis is modified to take the fixed charges into account. In the second phase, vectors are forced into the basis even though they increase the total cost, in the hope that, by resuming simplex iterations from a new extreme point, a better solution can be found.

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INCENTIVES FOR WASTE COLLECTION BASED ON WORK CONTENT MODELING

Richard L. Shell, P.E.
Professor of Industrial Engineering

Dean S. Shupe, P.E.
Associate Professor of Mechanical Engineering

UNIVERSITY OF CINCINNATI
Cincinnati, Ohio 45221

ABSTRACT

A successful incentive system for solid waste personnel must satisfy both technical and political requirements. The technical requirement is that each route assignment must contain a known collection work time. This paper describes the use of computerized modeling to develop waste collection route areas for either time or wage incentives. A recommended wage incentive program for solid waste workers is included with a simple example to illustrate application. The recommended program features an "Elective Incentive Contract" that combines three basic concepts: incentive teams, time and wage incentives, and elective work loads, i.e., teams choose their level of incentive work load.

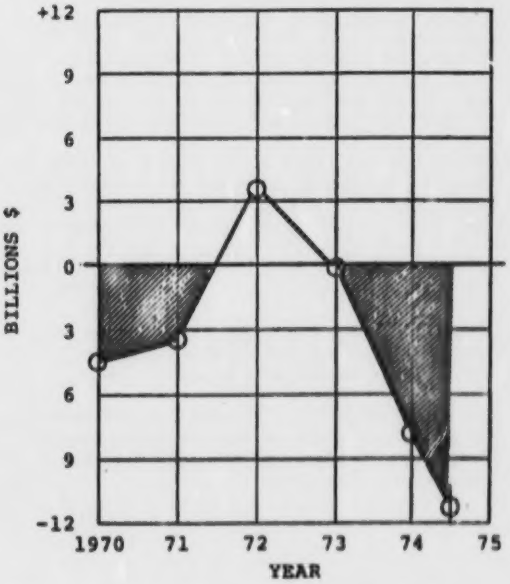
INTRODUCTION

Service cut-backs, layoffs, reduction in capital investments, and possible financial default -- these headlines evidence the growing economic plight of many cities across the nation. The typical municipality is being hard pressed to maintain its service-oriented, labor intensive functions in the face of continuing inflation while on a relatively fixed income base. "Over the past two decades, state and local spending, now running at $221.5 billion, has grown faster than any other sector of the economy. State and local expenditures, exclusive of federal aid, rose from 7.4 percent of gross national product in 1954 to 11.6 percent last year"[1].

The revenues of local government have not kept pace with the spiraling expenditures. The bottom line result to date has been deeper budget deficits. Figure 1 illustrates the worsening financial condition since 1973.

PRODUCTIVITY AND SOLID WASTE COLLECTION

In most cities, solid waste collection ranks third in total cost, behind education and roads. Collection has been traditionally noted for its intensive labor requirements. Typically over 70 percent of collection/disposal costs are required for collection manpower. Collection productivity has remained essentially unchanged since the introduction of the compactor truck nearly four decades ago. One approach to increasing productivity is the application of worker incentives.



Source: U.S. Commerce Department

FIGURE 1. STATE AND LOCAL GOVERNMENT BUDGET SURPLUS/DEFICITS

WORKER INCENTIVES

Any compensation offered for improved performance or behavior is an *incentive*. Incentive plans can be divided into three broad categories: direct monetary, indirect monetary, and non-monetary [5]. Under a direct monetary plan, each employee is compensated directly for his or her output or increased output. Direct plans can be either individual or group. Under the group plan, each member of the group is compensated an equal percent of bonus for the group's increased output.

A study of over 400 companies of all sizes to determine the effect on productivity of work measurement and wage incentives indicated that productivity in plants with wage incentive plans was 42.9 percent higher than plants with measured day work alone, and 63.8 percent higher than plants with no measurement [3,4]. These surveys indicate that a key to increased productivity is work measurement. "Without measurement, we don't know where we are or where we're going"[6].

Although monetary incentives have been utilized in manufacturing industries for several decades, their application to the service-oriented sector of the economy has traditionally been limited. The recent shift in the economy from manufacturing to services has been accompanied by a growing interest in the use of incentive programs for service-oriented public employees as recently reported by the National Commission on Productivity and Work Quality [2].

SOLID WASTE SYSTEM REQUIREMENTS

A wage incentive program for collection personnel must satisfy two major requirements: *technical* and *political*.

A sound technical base is fundamental to an incentive program. Each route assignment must contain a known collection work content, i.e., the work time required to accomplish a given task at a normal work pace. In waste collection, work content is the standard time required for completing the collection assignment, properly allowing for variations in tonnage, haul distance, equipment, crew-size, and other influencing variables. The work content must be accurately calculated utilizing work measurement techniques [10].

The second major requirement is political in nature. All involved parties -- elected officials, citizens, public works management, and workers/union -- must be amenable to the concept of time and wage incentives. On an on-going basis, management must continue to support the program fairly, e.g., defend the program to the citizens and to municipal employees not included in the incentive plan, and maintain competitive base earnings. In addition, all parties must be willing to share the savings resulting from increased productivity.

TEAM TIME INCENTIVES

Several constraints are inherent in solid waste collection effect system design and modeling. These include 1) the daily collection route is fixed, 2) the daily work content is variable, and 3) the work is typically accomplished by crews.

If each collection route is to be picked up consistently on its scheduled day, provision must be made for handling the fluctuations that inevitably occur in the work content of a collection area from day to day. Management has only two alternatives for dealing with these variations: either make changes in the resources assigned to the task, or allow the time required for the task to vary into overtime or into 'undertime' (in which case the men would be idle a portion of the day).

Generally, municipalities tend to avoid overtime, electing instead to permit the crews to complete their assignments early. If the workers are allowed to leave on completion of their assignment and are paid for a complete day, the program provides a time incentive (the 'task system').

Although time incentive programs are frequently used and offer advantages to both management and workers, they require balanced work assignments for cost effectiveness and fairness to individual employees [12]. On a day-to-day basis, balanced work assignments are difficult to maintain between individual crews due to uncontrollable factors, especially sudden equipment failure [11].

An approach used by some municipalities to reduce the inequities between individual crews is to group several crews together into a team under the field supervision of a foreman [7]. The team approach not only provides a mechanism for dealing with daily fluctuations in the work loads of its member crews but also tends to average out inevitable changes in waste generation patterns occurring in a dynamic city, thereby requiring somewhat less frequent route revision [9].

WASTE COLLECTION ROUTE DEVELOPMENT

In the development of waste collection routes, it is recommended that each route assignment be specified by a bounded geographic area. Detail sequential routing within the assigned area is best accomplished by public works management and collection personnel utilizing their experience and knowledge. Typically, a collection area consists of only a few square blocks, thus permitting heuristic design by collection personnel. In addition, most motivation and job performance investigations indicate that workers perform at higher overall productivity levels if they have been involved in the design and planning of their work activities. Therefore, detail sequential modeling of waste collection, e.g., the Chinese Postman, Eulerian Tour, and Traveling Salseman algorithms, has little practical value.

Route area development requires partitioning of the city into team and crew collection areas each defined so as to provide the desired work day. The total work content for each area must account for all work time elements: the sum of the pickup times as computed for each block, disposal time, refueling time, allowance for unavoidable delays, and worker rest breaks.

The development of route areas through modeling requires a knowledge of all work content time elements. Fundamental to the determination of pickup times for each block is detailed block-by-block field data on all variables influencing collection times and tonnages. This data includes setout containerization, street width and street length, and may be obtained by field survey teams that accompany crews during collection.

Utilizing the route area concept based on work content modeling, new collection routes were developed and implemented for Covington, Kentucky. Covington has a population of over 50,000 and is located in the Greater Cincinnati metropolitan area.

Based on the block-by-block data for Covington, together with work measurement results, predictive equations were developed for calculating the standard collection time for every block in the City. Times for the other work content elements were obtained by direct field timing and work sampling.

A system of simulation programs incorporating all of the work time elements was utilized to design collection route areas for the City. The programs were user-oriented with remote terminals linked to an IBM 370/168. Fixed inputs included collection frequency, crew size, and length of work day. Variable inputs included individual block identification numbers and map distances. Detailed outputs included all clock times and load tonnages as each truck progressed through its work day (reference Appendix A for example printout). Final output defined the number of truck crews required for collection of the entire City. In addition, balanced route area assignments were determined for individual truck crews, as shown in Figure 2. This type of route development provides the technical basis for a wage incentive program.

A RECOMMENDED WAGE INCENTIVE PROGRAM FOR SW WORKERS

If the technical and political prerequisites can be satisfied, an effective wage incentive program may be developed that offers high probability of long term success. A wage incentive program that lends itself particularly well to solid waste collection in medium and larger cities combines three basic concepts: incentive teams, a time/wage incentive, and elective work loads. It will be referred to as an *Elective Incentive Contract (EIC)* program[8].

Incentive Teams

Under EIC, collection is accomplished by incentive groups or teams consisting of approximately three to nine trucks and their assigned crews supervised by a field foreman. All supportive SW personnel including maintenance and disposal workers as well as the superintendent receive an incentive bonus based on the average of all teams.

Time Incentive

Each team is assigned a collection route area consisting of a standard work day (e.g., 6.5 hours average) that is less than the normal 8-hour day. Team members are paid for the full day and are permitted to leave work after their respective team area has been collected to the satisfaction of their field foreman. The time incentive encourages workers to reduce their collection time by increasing the work pace, reducing break time, or through worker ingenuity.

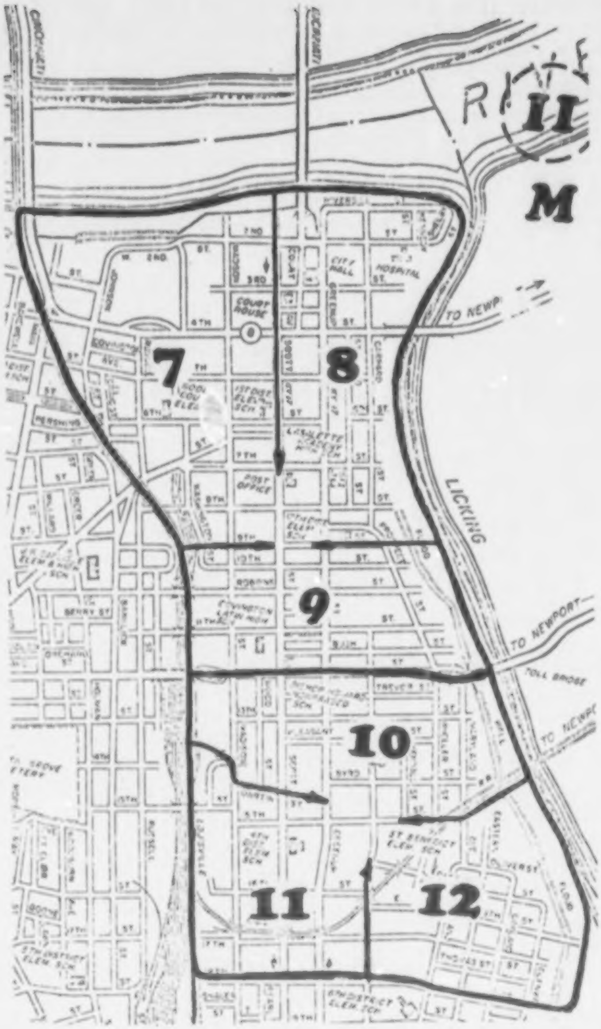


FIGURE 2. AREA ROUTE ASSIGNMENTS FOR TEAM II (TRUCKS 7 THROUGH 12).

Elective Participation

In addition to the 6.5-hour standard work day, individual teams may elect to contract additional work content in return for a wage incentive bonus. The bonus is based on an equal sharing by workers and city of the resulting savings.

EIC EXAMPLE

To illustrate the EIC program, consider a small solid waste collection/disposal system with two collection teams, both teams initially consisting of five rear-loading packers and drivers, five laborers, and a field foreman. Team I contracts the standard 6.5-hour work day and receives base salaries without a wage incentive bonus. Team II contracts for a 7.5-hour work day and receives base salaries plus a wage incentive calculated by the simple equation below:

$$\text{Wage Incentive (percent)} = \frac{(\text{Contract} - \text{Standard Day})}{8\ \text{Hours}} \times 100$$

For a 7.5-hour contract day, the computation is:

$$\text{Wage Incentive (percent)} = \frac{(7.5 - 6.5)\ 100}{8.0} = 12.5\%$$

In the case of a Team II worker earning a base salary of \$200 weekly, the resulting wage incentive bonus would be \$25 weekly.

A 7.5-hour contract work day for the 10-worker team reduces the equivalent manpower requirements for the total system by:

$$\text{Manpower Reduction} = \frac{(7.5 - 6.5\ \text{hours/worker})\ 10}{6.5\ \text{hours/worker}} = 1.54\ \text{workers}$$

Assuming a 30 percent overhead (including fringe benefits), the manpower reduction savings resulting from the 7.5-hour contract work day are:

$$\text{Manpower Reduction Savings} = (\$200/\text{week})(1.54) \times (1.30) = \$400/\text{week}$$

Net labor savings to the city is equal to the manpower reduction savings less bonus payments to team workers, foreman, and supportive personnel. Bonus payments to the workers of Team II would amount to \$250 (10 workers @ \$25 each). Assuming that bonus payments to the foreman and support personnel amount to \$50, the net labor savings to the city would be:

$$\text{Net Labor Savings} = \$400 - \$250 - \$50 = \$100/\text{week}$$

In addition to labor savings, the city would realize equipment savings associated with the reduction in manpower. For each crew reduced (2 workers), there is a reduction of one truck. Assuming a weekly truck cost of \$200, the equipment savings would be:

$$\text{Equipment Savings} = \frac{1.54}{2}\ (\$200/\text{week}) = \$154/\text{week}$$

In this example, total weekly savings to the city equals \$254 while the total weekly bonus payments to workers (including foreman and support personnel) equal \$300. Obviously truck and manpower reductions can occur only in integer units.

Since under the EIC program, the work groups contract to complete their elected collection assignment, overtime pay is avoided except for scheduled holidays. Care must be exercised during implementation of collection improvements to avoid employee layoffs if at all possible. Consequently, actual savings may lag implementation until manpower levels are adjusted through attrition or reassignment.

CONCLUSION

The findings from this project indicate that a wage incentive program for municipal solid waste personnel is feasible and technically possible, but that political problems more complex than found in private industry must be dealt with.

The recommended Elective Incentive Contract (EIC) program is based on carefully defined truck route areas with work content determined from computerized modeling based on detailed field data and work measurement techniques. Incentives are paid to small groups electing work content levels above standard. Savings resulting from increased productivity are shared equally between worker groups and management, and the municipality.

ACKNOWLEDGEMENTS

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APPENDIX A. SAMPLE COMPUTER OUTPUT OF ROUTE DESIGN SIMULATION, TEAM I.

```
RUN NEWMOD1

NEWMOD1      14:49   02/07/76  SATURDAY

DO YOU WANT ABBREVIATED OUTPUT?
    YES=1
     NO=0
?1

 IS IT A NEW ROUTE?
    YES=1
     NO=0
?1

 PLEASE PUNCH THE ESTIMATED MAP-DISTANCE IN IN
 FROM THE GARAGE TO THE FIRST STOP
?26

 TIME AT THE FIRST STOP IS  8:18

 ALLOWING 8.0 MINS. FOR FUELLING
 CLOCK TIME IS  8:26
```

```
NOW GO AHEAD AND START PUNCHING THE ID'S

 ID #
?4+341

          11.4      1083      8:37
 ID #
?342

          23.9      2220      8:50
 ID #
?344

          38.9      3713      9: 5
 ID #
?351

          58.3      5835      9:24
 ID #
?353

          69.7      6888      9:35
 ID #
?354

          83.8      8339      9:49
 ID #
?360

          98.6      9628     10: 4
    **** THE LOAD IS FULL ****
 PLEASE ENTER THE DISTANCE IN MAP-INCHES FROM
 THE LAND-FILL

?24

    THIS LOAD WEIGHS   9628 POUNDS
    TOTAL WEIGHT IN THE ROUTE =  9628 POUNDS
    TOTAL TIME IN COLLECTION =  98.6 MINS.
    TIME SPENT IN TRAVELLING = 34.1 MINS.
    TOTAL COLLECTION TIME IN THE ROUTE =   98
    TIME SPENT AT THE LAND-FILL = 10.0 MINS.
    CLOCK TIME IS 10:48

 ID #
?3

         111.9      1357     11: 1
 ID #
?4

         144.8      4900     11:34
 ID #
?4

    ****WARNING **** WARNING **** WARNING ****
 ID #     4 WAS ENTERED AS ITEM #   9 IN THE RC
 PLEASE ENTER OTHER ID# AGAIN

 ID #
?6

         149.9      5373     11:39
 ID #
?7

         156.3      6046     11:45
 ID #
?8

         163.0      6720     11:52
 ID #
?9

         175.6      7349     12: 5
 NOW IT IS TIME FOR THE LUNCH. WE SHALL
 ADVANCE THE CLOCK BY 30 MINUTES.
```

PLANNING FOR VARIATIONS IN SOLID WASTE GENERATION

Donald Grossman, Graduate Student
Civil Engineering Systems Laboratory
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Summary

A methodology developed for analysis of municipal solid waste collection explicitly plans for variations in waste generation. Using the method, a variety of district size, truck size, and crew size alternatives can be evaluated in a multiobjective framework, based upon a probabilistic description of overtime requirements. The methodology is applied in a case study for Warwick, Rhode Island.

Objectives considered in the case study included economic efficiency and the fraction of days requiring overtime. The model uses the historical distribution of district waste generation to forecast variations in waste generation as a function of district size. Collection productivity for a variety of truck and crew combinations is also forecast. System alternatives are evaluated analytically. The output provides a basis for choice by explicit representation of the tradeoffs between objectives.

Resource Allocation Decisions

Selection of truck, crew, and district size is a key element in municipal solid waste management. This research investigates these resource allocation decisions and develops a model to forecast the tradeoffs between objectives for alternative planning policies.[2] The resource allocation decision variables are isolated at the primary controls on collection available to local system managers. A variety of other controls are possible, but these are typically constrained by environmental factors or decisions taken over a longer time horizon.

The choice of truck size is one principle resource decision. Capacity, given district sizes, crew sizes, and a processing site configuration, determines the expected frequency and total duration of haul. As capacity increases, there are increased costs due to large truck sizes, but these trade off in savings in crew and vehicle costs due to decreased frequency of haul. Secondary effects from choosing large vehicles are a limited turning ability and less queuing at processing sites.

The choice of crew size is the second principle resource decision. Increased crew size, given truck size, district size, and a processing site configuration, results in expected decreases in overtime; these trade off against expected increases in fixed hour labor costs and in nonproductive haul time. Secondary considerations are crew safety and crew comfort; also, labor relations or political considerations may act to constrain the available crew sizes. Note that recent practice supports one to three member crews.[5]

The choice of district size, and therefore the number of trucks and crews required for collection (assuming one truck and crew per district), is the third principle resource decision. A priori, the number of districts, and therefore the number of trucks and crews, likely has the greatest impact upon system performance. Larger district sizes imply a smaller number of districts, and therefore fewer trucks and crews to service a given town. For a fixed truck and crew size, larger districts result in an expected decrease in capital costs because fewer resources are required, but these trade off against increases in truck and crew operating costs due to longer expected work days.

The above exemplifies some of the cost tradeoffs in resource allocation. The problem is framed as a supply problem with trucks and crews as inputs. One objective to consider is cost. In addition, there is likely some disutility for excessively long collection days, and thus suggests that the system manager might want to consider multiple planning objectives.

Waste generation is not deterministic. Assuming a constant rate of collection, the length of the collection day varies, and this induces a variation in the cost and other objectives. In addition, costs associated to resources are not well behaved, but are realized in discrete increments. Resources themselves are also discrete. For example, crews are typically paid for 8, 9, 10, or 11 hour days, and not for continuous timesteps. Both the stochastic character of waste generation and the discontinuities in input cost can be modeled using the methodology of this research.

Methodology

This section presents a procedure for choosing a resource allocation alternative, readily adaptable for use by a local system manager. First, possible collection system objectives are proposed, including appropriate measures of effectiveness. Second, the set of alternatives to be considered is identified. Third, a structure is developed for the evaluation of proposed resource allocation alternatives. Fourth, a multiattributed utility framework is presented as a means of choosing between alternative collection system configurations.

The analysis assumes a single decision maker, and choice within a maximum utility framework. The most obvious objective is financial, measured in present value dollars. The case study has shown that dollar costs provide insufficient basis for choice. Using only dollar costs, the manager would always choose to operate very few small trucks, and prefer to pay large amounts of overtime. Instead, a second objective is to limit the expected length of overtime, expected number of days on which overtime is paid, or the expected number of days with one, two, three, or more hours of overtime. Modeling this objective affords the manager control of distribution and frequency of overtime hours.

The set of alternatives may be characterized as points in a three dimensional space. Truck size alternatives are based upon industry standards (e.g. 13, 16, 18, 20, 25 cubic yards) and limited only by technical considerations such as highway weight regulations. Crew sizes generally range from one to three members and may be constrained by union or similar considerations. District size alternatives depend upon the number of trucks and a design number of households. Generally, the number of districts will be a uniform multiple of the number of trucks (e.g. 1,2,3... trucks imply 5,10,15... daily collection districts).

The framework for evaluation of alternatives is an accounting scheme. The proposed method will yield analytic results. District size determines the number of trucks and crews. This, in conjunction with truck capacity and crew size, determines the regular costs paid on a fixed length workday basis, and the capital costs associated to owning the trucks and ancillary support facilities. This component of total system cost is deterministic and easily calculated. The other important costs are those for truck operation or overtime. The evaluation of these requires a description of the demand for collection services including the time variation of district waste generation. The evaluation also requires a model of the supply side, that is a model of the productivity of truck and crew combinations.

The waste collected from a residential waste collection district will normally vary greatly over time. The data from Warwick showed the magnitude of these excursions to be greater than 50 percent of the mean weekly wasteload measured in pounds. Three sources are expected to explain these variations. First, even after correcting for changes in the numbers of households, the data may exhibit a long range trend in waste generation rates. This suggests changing consumption/disposal patterns in the population as a whole. If the analyst has a sufficiently long record of weights, it is possible to remove the trend and later reintroduce it for an appropriate design year. Second, variations will normally be manifest within a single year due to seasonal consumption and disposal patterns. These arise because of sociological factors including vacations, habits, and economic trends, and because of natural factors including weather and climate. Again, if the analyst has a sufficiently long, trend free record, the seasonal variations could be removed by a technique such as Fourier analysis. Third, it is postulated that there is an underlying random component in household waste generation. The process need not necessarily be known, but the analyst must test whether, at the district level of aggregation, an arbitrarily chosen set of households exhibits the same waste generation character as any other district containing an equal number of households.

The following discussion assumes that the decision maker's purpose is to choose a single resource allocation. The importance of considering only a single allocation is that it enables the analyst to model the distribution of the quantity of waste generated for collection, without the need to model the relationship of different waste quantities over time. Specifically, the preservation of autocorrelation need not be considered.

The minimum data requirement to model time variation are weekly wasteloads from sample daily collection districts for a year, and the members of households for each observed district. If the wastes aggregated to the district level can be shown to be normal, it is possible to model the district wasteload as the sum of independent, identically distributed waste generation distributions. The household distribution independence and form cannot be tested with available data. It is possible, however, to arbitrarily choose to model individual households as normal, and, as long as a reasonable number are aggregated into districts, the normal distribution in district level waste, if substantiated by the data, can be preserved. For the case where observed districts have an average of k households

$$\hat{\mu} = n\ u \qquad (1)$$

$$\hat{\sigma}^2 = k\ n\ s^2 \qquad (2)$$

where n is the number of households in the district size alternative to be forecast, and u and s^2 are the estimated parameters assumed to characterize the normal distribution on wastes generated for collection by individual households. Using the model of equations (1) and (2), the demand for waste collection services for a range of district size alternatives may be forecast.

The second concern is to describe the productivity of various crew and truck size alternatives for the set of proposed district size alternatives. To relate these to system objectives, total collection time must be predicted for forecast wasteloads, and, in turn, these collection times can be translated into expected cost and other systems objectives. For a particular district size, consider the examination of t_1, t_2, t_3 ...t_k length workdays (for example 8, 9, 10, and 11 hour days). The discretization should correspond to cost increments. Corresponding to these times are maximum collectable wasteloads, call these w_1, w_2, w_3, ...w_k, for each truck and crew alternatives.

The total workday may be characterized as the sum of on route collection travel (from garage to and from route, and from route to processing or disposal site), and nonproductive time (breaks, breakdowns, and maintenance). Typical values for nonproductive time may be estimated. The number of hauls and on route collection time depend on wasteload, truck size, and crew productivity. To complicate this analysis, trucks are volume constrained. Therefore, an expected density of waste is required to convert volumetric capacity of each truck size alternative to a corresponding weight capacity. The procedure for estimating density is to use observed data points having more than a single haul to the processing site, and assuming the first haul full. Then the analyst can estimate density using known truck weights and volume. In the Warwick case study, a point estimate of density was justifiable.

Shuster[4] has developed and calibrated a model to forecast Y, the service time per household, in minutes. The regression equation, estimated for a curbside, once weekly, incentive system is

$$Y = .0088\ x_1 - .0570\ x_2 - .0010\ x_3 - .0423 + .770 \qquad (3)$$

where x_1 is the pounds of waste per service per week, x_2 is the crew size, x_3 is the percent one-way items, and x_4 is the collection miles per day. Shuster estimates similar models for other levels of service and work rules. Therefore, for each resource allocation alternative, the on route collection time may be forecast for all levels of w_k. Under an assumed waste density, the number of hauls and the corresponding travel times may also be determined. Then, for each resource allocation alternative, the analyst has determined each w_k associated to each workday length t_k. It is important to note that productivity is assumed to be deterministic, and more research is required to test the validity of this assumption.

Therefore, for each resource allocation alternative, the distribution on wasteloads yields a distribution on the total length of collection day. Given estimates of cost for varying length collection days, the expected cost of collection and values for other objectives may be developed. The levels of attainment of objectives can be represented by points on a transformation curve. The decision maker's problem is to choose between alternative operating points along the transformation curve. The chosen point is the desired level of tradeoff between system objectives. It should represent the alternative with the greatest utility to the system manager. Choice can be made subjectively, from a graphical representation, or can be made in a multiobjective framework as described by Keeney[3], and others.

Case Study - Warwick, R.I.

The resource allocation methodology was applied in a case study for Warwick, R.I. First, Warwick and the available data sources are described. Second, the key steps and results of the evaluation process are presented. Third, output under a variety of assumptions and system objectives is presented. Finally, tentative resource allocation policy recommendations are drawn.

Warwick is a moderately large community with a 1970 census count of 83,694 people. The municipal Public Works Department provides collection from residences: there are nearly 24,000 dwelling units serviced in public collection. At the time of data collection, eleven 20-yard loadmaster compactors were the town's primary collection vehicles. The vehicles were operated by three member crews paid on a 40-hour incentive system, with overtime paid at time and one-half. Data were collected by ACT Systems[1] for 20 of Warwick's collection districts for the entire period from November, 1972 to November, 1973. Data collected included total weekly wasteloads, and the respective numbers of households in each of the districts. Disaggregation to weight per haul enabled estimation of waste density. The data used for the Warwick case study represent a minimum set necessary for analysis.

The 20 timestreams of 52 observations in weekly district waste generation contained only 996 non-zero observations. These, average weights per household per week were calculated. A week test suggested that all producers behaved as if drawn from a single population. Using the 996 observations as independent samples from a distribution on average household wastes, then the hypothesis that the underlying distribution is normal may be tested. Independence of samples was screened by checking correlation statistics across districts, the estimated sample parameters for the distribution were a mean of 61.63 pounds and a standard deviation of 18.42 pounds. In addition, a 'minimum correlation sample of 52 observations produced essentially the same distribution parameters. Using a Chi-squared goodness of fit test, the hypothesis that the samples came from a normal distribution with the estimated parameters could not be rejected. Using the sample parameters, distributions in waste generated were forecast for district size alternatives ranging from 270 to 600 households per district.

The modeling of waste collection time used Shuster's regression equation. In addition three-quarter hours of official breaks were assumed. The garage and processing site are at the same location, and were modeled as equidistant from all districts. Only the three member crew size alternative was tested. ACT Systems data reported 72 percent one-way items and also reported data which were converted to collection miles per household. Using the model of equation (3), the total collected wasteload w_e, for each level of time, t_k, could be forecast.

Five commercially available truck size alternatives were selected. Capacities ranged from 13 to 25 cubic yards. The mean density of waste used to convert volumetric capacity to weight capacity was 666 pounds per cubic year. The assumed discretization of costs were those associated with 8, 9, 10, and 11 hour long days. These were converted to probabilistic equivalents. Table 1 shows the model output for a 20 cubic yards truck, with a three member crew, operating in a district of 480 households.

P_1 = Prob ($t \leq 8$ hours) = .73

P_2 = Prob ($8 < t \leq 9$) = .20

P_3 = Prob ($9 < t \leq 10$) = .04

P_4 = Prob ($t > 10$ hours) = .03

Table 1: Sample Distribution on Collection Day Length

The model forecasts that roughly 73 percent of the days have collection times less than 8 hours. Similar information may be inferred for all other resource allocation and day length alternatives.

Two objectives were chosen for the Warwick case study. One proposed objective is the cost for each system alternative, measured in dollars; costs include regular, capital, operating, and overtime components. In a supply model framework the dollar benefits should be the same for all supply alternatives. The second proposed objective, the fraction of days exceeding 8 hours in length, provides some measure of the disutility of overtime incidents not captured by the dollar costs. Resource allocations having both lower cost and lower fraction overtime requirements are preferred.

The expected fraction of workdays exhibiting overtime is easily developed from information such as that in Table 1. Standard cost data collected by ACT Systems were used in the assessment of system costs. For the Warwick case study, a single year planning horizon was modeled in order to assure comparibility with the historical data. Costs were normalized to dollars per ton. Figure 1 shows the tradeoffs between the attributes of the system objectives.

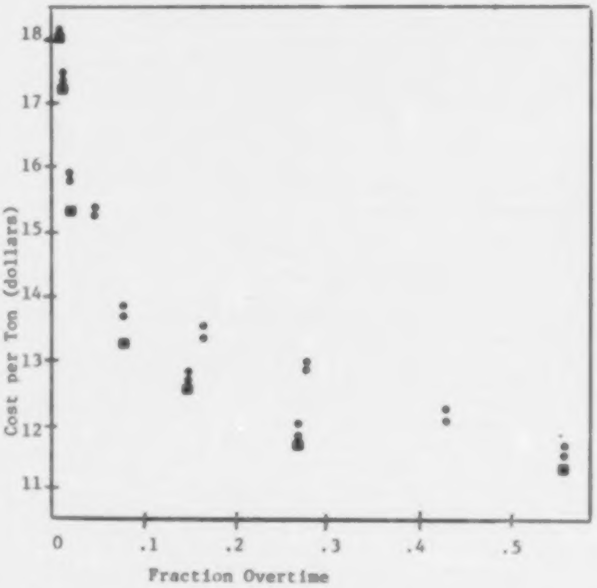

Figure 1: Attribute Transformation Array

Each point represents a distinct resource allocation and shows the levels of attributes forecast for that alternative. A southwest corner rule identifies non-dominated alternatives. These are the circled points in the figure.

The actual choice of objective requires preferences for tradeoffs between objectives. The past Warwick resource allocation shows implicitly the preferences between objectives. In 1973, Warwick used eleven 20-yard trucks with three member crews. The model forecast for Warwick's chosen alternative was collection costs of $12.75 per ton, and overtime paid on 15 percent of the workdays. The actual Warwick system, using the historical records from November, 1972 to November, 1973 exhibited collection costs of $12.82 per ton. The model forecast falls within one percent of the actual system cost. No historical data on the actual distribution of overtime were available.

Actual validation of the forecasts is difficult. A plausible technique is testing the sensitivity of the chosen alternative to the input assumptions. To illustrate, this research tested changes in overtime and wage rates. The effect of different overtime rates could provide information for a negotiation process. For Warwick, double, and even triple normal wage rates for overtime resulted in only minor cost advantages for larger trucks. Higher overtime rates had greatest effect for alternatives with a greater expected function of overtime, but overall fixed hour wages and base truck costs dominated total system costs. Similarly, doubling regular wage rates had little effect on the least cost system alternative; this suggests that wages already dominated the total costs.

In general, the Warwick Case Study shows that the actual 1973 collection system had evolved to represent a fairly reasonable tradeoff between the investigated alternatives. Observe that low overtime alternatives result in significant cost increases. For the total system, the model forecast approximately a one-quarter million dollar increase in costs by changing from a 15 percent to a no overtime alternative. Due to the variability in the district waste generation, planning for even moderate amounts of overtime is likely advantageous. Whenever possible within the context of overtime considerations, fewer and larger districts are preferable. Total system costs seem relatively insensitive to truck costs: labor costs dominate. This suggests the choice of larger trucks, but, beyond a certain size, additional capacity affords little cost advantage because the expected number of hauls do not decrease further. In any case, the resource allocation methodology applied to Warwick provides a wealth of information conveniently represented and useful for decision making.

Conclusions

The resource allocation proposed in this research incorporates multiobjectives, uncertainty, and nonlinearity. It is not an optimization procedure: there is no directed search towards most preferred alternatives. Instead all alternatives are simulated, analytically, and exhaustive search is used to choose the resource allocation. A more detailed simulation is possible, but this would require more extensive data and might be a useful tool for testing the method. Nonlinear vector optimization using mathematical programming is also possible, but the formulation would be difficult, and integer constraints might make the solution impossible. In light of the relative ease of application of the method, and the importance of certain modeled system characteristics, the resource allocation procedure of this research seems effective for the planning of municipal collection services.

Several extensions are possible. The analyst might model changes in the underlying waste generation process through trend extrapolation, or alternatively through causal modeling of the waste generation process. The latter is currently beyond the state of the art. Alternatively, seasonal allocations of resources instead of a single level of resource allocation might be developed. Different seasons appear to have different waste characteristics. Therefore, seasonal allocation, facilitate better matching of supply to the demand for collection services. Tests with Warwick data indicate that each season can be modeled as described in this paper, and a dynamic programming formulation used to coordinate the seasonal allocations to maximize overall system objectives. Another extension, requiring more research, is modeling several populations of waste producer. One possible approach is to partition the populations into separate subsystems.

The potential gains due to the use of an analysis model of the type developed are significant. The method is easily applied to local collection system planning. Analysis helps identify and clarify the framework and assumptions of the decision process, and provides a basis for testing and comparison of alternative decision strategies. The method, using easily available data, tests and can model a variety of important process characteristics, test a variety of input assumptions, and lend valuable insight into the tradeoffs between system objectives under alternative resource allocations.

Acknowledgements

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MODEL OF THE MOVEMENT OF HAZARDOUS WASTE CHEMICALS FOR SANITARY LANDFILL SITES

Eugene Elzy
Department of Chemical Engineering
Oregon State University
Corvallis, Oregon 97331

F. Tom Lindstrom
Departments of Statistics and Mathematics
Oregon State University
Corvallis, Oregon 97331

Summary

A simple mathematical model has been developed to aid in the management of hazardous chemical disposal in sanitary landfill sites. The model is based upon a chemical mass balance and incorporates the important physical-chemical parameters: 1) hydrodynamic flow velocity based upon the porosity and hydrodynamic gradient of the porous medium; 2) variable water table; 3) variable rainfall; 4) reversible adsorption-desorption phenomena; 5) first-order irreversible sorption, if any; 6) first-order chemical reaction; and 7) first-order microbial degradation kinetics. The chemical, which is deposited into the landfill in any time pattern desired, is routed vertically by rainfall infiltration to the water table where movement in the horizontal direction occurs. The simplicity of the model and the resulting computer simulation program permits a ten year run to be computed and plotted automatically for approximately sixty dollars. The application of the model for a typical sanitary landfill is demonstrated.

Introduction

In determining whether a specific material is environmentally hazardous under a given disposal situation, a number of factors must be considered. Important material properties or characteristics include toxicity, solubility, biodegradation rate, vapor pressure, adsorption on soil, amount, concentration, and others. Other important factors include containment and geologic or hydrologic conditions of disposal.

In only a few instances can the environmental hazard of disposal of a certain material be defined on the basis of only one or two of the factors mentioned above. In most cases it appears necessary to consider many factors and consequently hazard evaluation may become quite complicated. The major threat to the environment presented by the disposal of hazardous or toxic chemicals in sanitary landfill disposal sites is contamination of ground water or surface water. In order to predict potential ground water or surface water contamination it would be necessary to consider all important physical and chemical characteristics and environmental conditions (geologic and hydrologic) at the same time by a mathematical approach.

A review of the literature reveals numerous papers dealing with the mathematical aspects of water and chemical movement in both unsaturated and saturated porous media. Extensive mathematical modeling and computer simulation studies of regional ground water flow have been performed by Freeze[3,4]. He considers the interaction between a pollutant source and the soil-moisture and groundwater flow systems. The Freeze model can predict both transient and steady state subsurface flow patterns in two or three dimensions and includes consideration of both saturated and unsaturated zones. Quantitative interpretation of Freeze's results provides predictive values of the rate of entry of pollutants into the flow system, lengths of flow paths, travel times of pollutants, discharge rates to surface water, water table movements, and pressure field development. These results do not consider dispersion or hydrochemical interactions between pollutants and soils.

Pinder and coworkers[6,7] have also developed sophisticated two and three dimensional models of ground water flow systems, including mass transport in flowing ground water. Schwartz[9] considered the simulation of hydrochemical patterns in regional ground water flow.

In this sanitary landfill modeling project, constraints of time and funds virtually eliminated consideration of modeling using the techniques of the above workers. For example, Freeze[3] reported that transient two-dimensional hydrodynamic models required from 10 to 30 minutes of computer time (IBM 360/91) for 100 time step solutions. Since the current project requires a simulation of the landfill behavior over a time period of years, it is obvious that computer charges would be prohibitive for routine use of the model.

For practical reasons, a simple approach was taken using the vertical moisture routing procedure of Remson et. al.[8], Fungaroli,[5] and Bredehoeft et. al.[2], coupled with a simple model of the chemical transport in the horizontal direction. The hydrodynamics are not computed. Constant horizontal water velocities in the landfill and soil are estimated from soil or landfill permeability and porosity and local hydraulic gradients. The water table variations are entered as input data and are obtained from measurements taken near the landfill site.

While this approach of using greatly simplified hydrodynamics has obvious inadequacies, the simple model should be useful for management of chemical disposal in sanitary landfills. The assumptions and simplifications utilized to construct the simple model result in higher predicted concentrations than is expected in actual disposal situations. Thus the model is conservative with respect to potential health hazard, a desirable approach to waste disposal management. Future comparisons of model predictions with actual sanitary landfill behavior will enable the model accuracy to be determined.

The SLM-1 Model

The objective of this project is to develop a computer model of a sanitary landfill which is as simple as possible and yet still include the principal factors affecting the underground transport of the contaminant:

At a minimum, the model must account for the following factors:

1. both vertical and horizontal movement of the contaminant (i.e. two dimensional distribution of chemical),

2. adsorption of the porous media,

3. biodegradation of the contaminants,

4. variable water table which may rise to any height in the landfill (possibly even completely flooding the landfill) or drop to a depth below the landfill,

5. permeability, porosity, hydraulic gradient and moisture bearing characteristics of the soil and landfill.

The sanitary landfill model SLM-1, developed in this study, is based on a vertical routing of contaminant by a method similar to Remsom et al.[8] and a horizontal routing corresponding nearly to flow through a series of stirred tanks. The model is greatly simplified by performing a mass balance on the contaminant only. No water balance is performed. The horizontal velocity of the groundwater is assumed constant in the landfill and soil and is estimated from the permeability, porosity, and the hydraulic gradient of each media. Both the landfill and the soil are assumed to be homogeneous with uniform permeability, porosity, hydraulic gradient, biodegradation, and adsorption characteristics within each porous medium.

Two-Dimensional Structure of SLM-1

The landfill and soil region is divided into a grid, each compartment having dimensions of length DELX, depth DELZ = 2 feet, and width WIDTH sufficient to encompass the contaminated zone of the landfill. SLM-1 is considered to be a two-dimensional model since calculations account for distribution of chemical in two directions only; i.e., vertical and horizontal. Since dispersion of chemical in a lateral direction is ignored, the model tends to calculate a higher concentration at a point downstream from the landfill than would exist if the three-dimensional dispersion character were modeled.

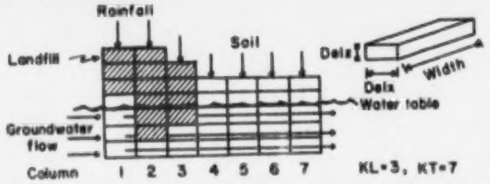


Figure 1. Two-Dimensional Structure of SLM-1

The elevation of the top of each landfill and soil column and the elevation of the bottom of each landfill column are specified as input data. It is assumed that columns 1 to KL are landfill columns followed by KL+1 to KT columns of soil where KL and KT are specified as input data. KL=0 means that the entire region is soil.

Water Movement

The horizontal groundwater flow below the water table is assumed to be unidirectional with a velocity V(1) ft/day in the landfill and V(2) ft/day in the soil. Movement of the chemical in the lateral direction is neglected.

Rainfall at an arbitrary rate R(J) falls on the landfill and soil region and a fraction XINFL is assumed to infiltrate into the porous media. This water moves downward in the columns according to the simple mechanism suggested by Remson et. al.[8]

Each two foot layer above the water table has an initial moisture volume fraction of YI(1) for landfill and YI(2) for soil. Water entering the top layer in a column is retained until a moisture volume fraction corresponding to field capacity is reached, i.e., YF(1) for landfill and YF(2) for soil. Additional water entering a layer at field capacity freely drains to the next layer below and so on. Eventually, all layers above the water table will reach field capacity. Additional water into the top layer will then move downward to the water table carrying the chemical contaminant into the groundwater. Each calculational time period is two days; thus, it is assumed that the porous media above the water table can drain from saturation to field capacity within this time.

Chemical Source

At time zero, the chemical contaminant distributed in any compartment of the landfill or soil columns is specified as M(I,K) grams (entered as input data) where I is the layer number and K is the column number. An arbitrary source S(I,K) of chemical can be specified for any layer I,K as a function of time period J. Groundwater flowing below the water table into column 1 and the precipitation entering the top layer of each column are assumed to contain no chemical contaminant.

Adsorption Characteristics

Reversible adsorption of the contaminant onto the soil and/or landfill material is assumed to be described by the Freundlich equation:

$$MA = K \cdot C \cdot SOLID \tag{1}$$

where: MA = chemical adsorbed (grams),
C = concentration of chemical in free solution (mg chemical/liter or ppm),
SOLID = grams of porous solid material,
K = adsorption constant; may be different for soil and landfill material (liter/gm solid).

Biodegradation of Contaminant

Biodegradation of the contaminant is assumed to be first order:

$$MC = k \cdot C \cdot W \cdot \Delta t \cdot 10^{-3} \tag{2}$$

where: MC = chemical degraded by reaction (grams),
k = rate constant (hr^{-1}); may be different for soil and landfill material
W = volume of solution under consideration (liters),
Δt = time period (hours).

Chemical Mass Balance

Layer Above the Water Table. Each layer receives leachate from the layer immediately above and discharges leachate of different concentration to the layer immediately below. The mechanism proposed for mass balance calculations for a two-day period is as follows:

The volume of leachate from Q_{in} liters, is added to the volume of liquid in the layer from the previous time period.

$$W = W_{old} + Q_{in}, \text{ with W and Q, measured in liters.} \tag{3}$$

The total grams of contaminant is computed.

$$M_{total} = M_{old} + Q_{in} \cdot C_{in} \cdot 10^{-3} + S, \tag{4}$$

where S is the source function, i.e., grams of contaminant added during this two-day period. The total grams of chemical now is considered to adsorb on the porous surface, to degrade by reaction or to remain in free solution.

$$M_{total} = MA + MF + MC \tag{5}$$

where: MA = adsorbed chemical (grams),
MF = contaminant in the free solution (grams),
MC = chemical degraded (grams).

Since $C = \frac{MF}{W}$ (1000), where C is the concentration in ppm, the equations can be combined to yield:

$$MF = \frac{M_{total}}{1 + \frac{K}{W} \cdot SOLID \cdot 10^3 + k\Delta t} \qquad (6)$$

The total grams of chemical in free solution MF, the free concentration C, and the grams of chemical degraded MC can now be calculated. If the volume of liquid in the layer exceeds that corresponding to field capacity, VFC liters, the layer is drained to field capacity, i.e., if $W > VFC$, $Q_{out} = W - VFC$, otherwise $Q_{out} = 0$. The loss of contaminant to the layer below $Q_{out} \cdot C \cdot 10^{-3}$ grams, is computed next. The total liquid in the layer is now reset to $W - Q_{out}$ and the total grams of chemical adjusted to $M = M_{total} - MC - Q_{out} \cdot C \cdot 10^{-3}$.

The layer collects the leachate from above, mixes, adsorbs, reacts, and then drains to field capacity to supply leachate to the layer below. Thus, the process proceeds.

Layer Below the Water Table. A layer below the water table has a horizontal flow input and output due to groundwater flow. It is assumed that the layer immediately below the water table receives all the chemical in the leachate which is routed vertically due to rainfall infiltration. This assumption implies that the landfill is located in a groundwater discharge area. Layers further below the water table do not distribute the chemical vertically.

A layer below the water table is saturated, i.e., $W = VSAT$. Horizontal routing is assumed to occur in the following way. QH liters of liquid flows from a compartment at concentration C ppm, thus $QH \cdot C \cdot 10^{-3}$ grams are transferred downstream to the next column in the same layer. QH = volume of liquid into the layer in a two-day period.

$$QH = V \cdot DELZ \cdot WIDTH \cdot 2 \cdot 28.32 \cdot YS \qquad (7)$$

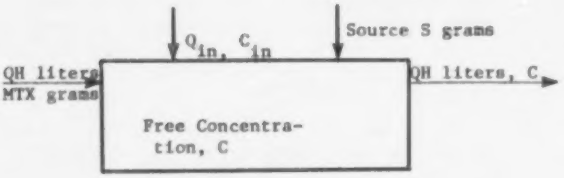
where: V = groundwater velocity (ft/day),

28.32 = conversion factor (ft^3 to liters),

YS = saturated volume fraction for porous media = porosity.

Source chemical (S grams), chemical in the groundwater from the layer immediately upstream (MTX) and chemical from the layer above (only for the first layer below the water table) are added to the layer.

$$M = M_{last\ J} - \underset{\text{(downstream)}}{QH \cdot C \cdot 10^{-3}} + \underset{\text{(upstream)}}{MTX} + \underset{\text{(above)}}{Q_{in} \cdot C_{in} \cdot 10^{-3}} + \underset{\text{(source)}}{S}. \qquad (8)$$



The total chemical now mixes, adsorbs, and is partially degraded. The total grams of chemical $M_{this\ J}$ is adjusted accordingly, $M_{this\ J} = M - MC$.

Variable Water Table

Rising Water Table. If the water table has risen since the last time period, it is assumed that the layers now saturated which were previously at field capacity (or lower) are brought to saturation with water having no contaminant. That is, bringing these layers to saturation has resulted in no movement of chemical. Then, calculations are performed to distribute the chemical vertically by infiltration and horizontally by groundwater flow as described earlier for the constant water table case.

Falling Water Table. When the water table drops, the layers at saturation capacity above the new water table must drain to field capacity which causes a vertical routing of chemical in a manner similar to the usual case for layers above the water table.

For calculational simplicity, the water due to rainfall infiltration and this excess water (VSAT-VFC) are routed vertically at the same time.

Validation of the SLM-1 Model

In the SLM-1 model, there are three major calculational procedures which should be validated.

1. Vertical routing of the chemical from the landfill or soil media to the water table, an unsaturated flow mechanism,
2. Horizontal distribution of chemical by groundwater flow beneath the water table, a saturated transport mechanism,
3. And routing of the chemical near the water table interface as the water table rises or falls.

Vertical Routing of Chemical Above the Water Table

The SLM-1 model uses the method of Remson et al.[8] to route moisture downward in the unsaturated media to the water table. These investigators have shown that this simple procedure satisfactorily agrees with experimental results in a laboratory landfill. The SLM-1 model extends the Remson procedure to chemical routing by assuming that each two foot layer of porous media acts as a well-mixed vessel in transporting the chemical downward. Although untested with experimental data, this procedure is expected to satisfactorily predict chemical movement above the water table, provided the soil can drain freely to field capacity in a two day time period.

Horizontal Distribution of Chemical in Groundwater Flow

To determine the validity of the SLM-1 model predictions of chemical movement beneath the water table, two auxiliary models were developed in this study.[11] A continuous one-dimensional model with an exponential source function and a multi-tank approximation of the continuous model were compared with SLM-1. SLM-1 predicts essentially the same horizontal distribution as the multi-tank model. Results from the multi-tank model approach the continuous model behavior as the tank size is decreased. It was concluded that the SLM-1 model agrees reasonably well with the classical model of one-dimensional species movement in a saturated porous media.

Variable Water Table Effect on Chemical Distribution

The model calculations for the case of a rising or falling water table have not been validated due to the lack of a satisfactory standard for comparison. Future studies should attempt to validate the assumed distribution mechanism.

Case Study

Brown's Island Landfill, Salem, Oregon

A general description of the Brown's Island area is included in the report by Balster and Parsons[1]. A complete report by Sweet[10] concerning the hydrogeology of the landfill site is on file with the Oregon State Engineer and the Department of Environmental Quality.

The Brown's Island landfill is located between the Willamette River and a meander channel of the river. It occupies the lowest geomorphic unit in the valley, the flood plain, and is subject to surface water inundation. Both the soils and the immediate subsurface deposits at the site have relatively high hydraulic conductivity.

Infiltrating precipitation and a water table which regularly saturates the putrescible material deposited at the site results in the generation of leachate at the site. The down-gradient flow of the leachate is sub-parallel to the flow direction of the adjacent surface water bodies. This results in the degradation of the shallow ground waters in the local system and the eventual drainage of some contaminants into the local surface water bodies, i.e. the sloughs, the ponds in the borrow pit bottoms, and the Willamette River.

A ground water monitoring system has recently been installed at the site. In the future it will be possible to monitor the quality of the groundwater in the vicinity of the landfill and to compare the observed leachate concentrations with those predicted by the model.

SLM-1 Model Calculations - Hypothetical Source

Figure 2 gives all the input data used in this case study. A typical annual water table elevation, in feet above mean sea level, of the Brown's Island area is shown. It was assumed that 45,400 grams of a chemical were initially distributed in an area 4 ft by 40 ft by 20 ft at the top of the landfill with no source added thereafter. The simplified rainfall and soil characteristics correspond to conditions typical of the Brown's Island area.

Figure 3 shows concentration distributions as a function of time at 400 feet down the hydraulic gradient from the landfill site. Observe that in all the cases shown in this figure that it takes at least three years before any appreciable concentration amplitude is obtained at the 400 foot distance from the landfill site. That peaks (pulses) of chemical concentration are generated and then dispersed while translating down gradient is a very real physical phenomenon and reflects among other things, the physical interplay of a pulse type annual rainfall and the variable elevation of the water table under both the landfill site elevation (chemical source) and the soil conduit. The explanation of the peak(s) formation is as follows. A portion of the rain that falls upon the surface of the landfill site penetrates the surface creating the potential for moving some of the chemical vertically downward according to the rules of moisture routing. Simultaneously, the water table is moving up and down. When enough water moving downward from the top of the landfill site (carrying some but not all of the chemical with it) meets the water table, then chemical moves horizontally and eventually out into the various soil conduits. Only four layers of soil conduits are shown in Figure 2. However, this is adequate to demonstrate the model. Once the chemical pulse reaches one of the soil conduits, it can continue to be distributed by convection and dispersion down gradient so long as the water table covers that conduit. When the water table drops below the level of that conduit then horizontal motion ceases and vertical motion is allowed to proceed according to the previously mentioned rules of the model. The net result, as might be observed in a monitoring well (impervious casing) bored through the top three conduit (layers) and into the fourth at the 400 feet down gradient point, is the concentration distribution curves shown in Figure 3. This figure demonstrates the effects that reversible linear adsorption and irreversible microbial degradation and/or first order chemical reaction would have on the concentration distributions.

Numerous computer simulation runs have been made for various source functions and for a wide range of adsorption-degradation conditions. All parameters of the model have been studied to demonstrate model sensitivity. Adsorption and degradation are the key parameters for predictive model calculations.

Each computer run of ten year duration costs approximately $60 using the Oregon State University CDC 3300 computer, including the plotting of all results. The model is usually run from a remote location by timesharing with the results plotted on a graphics terminal for ease of interpretation.

Recommendations

It is believed that this rather general predictive model for the movement of hazardous waste chemicals in both the landfill and the surrounding porous medium is valid enough to be used as a decision-making tool in the management of hazardous waste disposal. It clearly sets the upper limits on the expected concentrations for a real field situation. However, the complete model should be given a long-term field test. This field test might be carried out by incorporating a sufficient number of monitoring wells together with known charges (geometric position and actual chemical mass known at the time of introduction) of certain industrially and agriculturally important chemicals, which may typically be dumped into a landfill site. While the model is composed of generally field-tested components (vertical routing techniques worked out at Drexel University by Remson et. al.,[8] and horizontal saturated flow techniques well-known in chemical engineering), this particular model which combines both the vertical and horizontal techniques has never been field tested.

Acknowledgement

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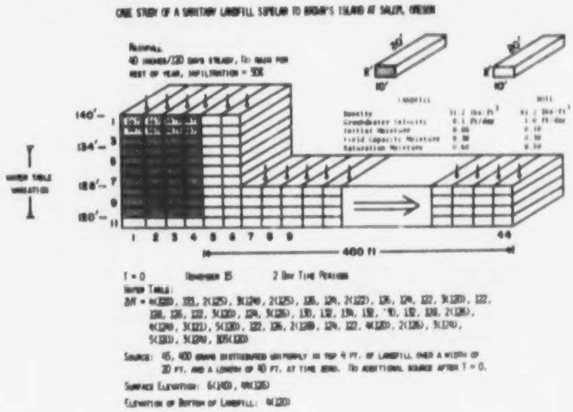
CASE STUDY OF A SANITARY LANDFILL SIMILAR TO BROWN'S ISLAND AT SALEM, OREGON
RAINFALL
INFILTRATION = 50%
LANDFILL
SOIL
Density
Groundwater Velocity
Initial Moisture
Field Capacity Moisture
Saturation Moisture
140'
134'
120'
WATER TABLE VARIATION
1
2
3
4
5
6
7
8
9
44
400 ft
T = 0
2 DAY TIME PERIODS
WATER TABLE:
SOURCE:
SURFACE ELEVATION:
ELEVATION OF BOTTOM OF LANDFILL:

Figure 2. A Case Study of Brown's Island Sanitary Landfill

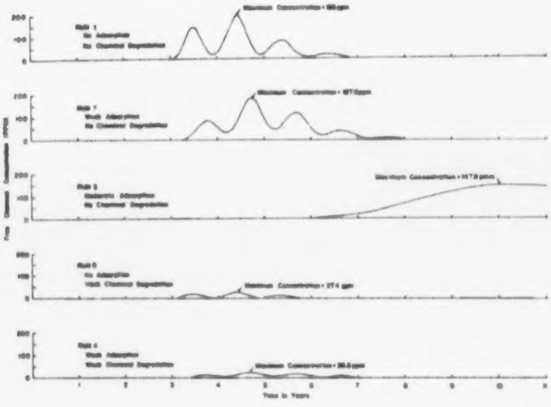

Figure 3. Typical Concentration Plots at 400 Feet Fro the Landfill

PHYTOPLANKTON BIOMASS MODEL OF LAKE HURON AND SAGINAW BAY

Dominic M. DiToro
Environmental Engineering and Science Program
Manhattan College
Bronx, New York 10471

Walter F. Matystik, Jr.
Environmental Engineering and Science Program
Manhattan College
Bronx, New York 10471

Summary

The basis for this analysis and projection of Lake Huron and Saginaw Bay phytoplankton biomass is a dynamic mathematical model which relates the growth and death of phytoplankton biomass to the nutrient concentrations on the one hand and zooplankton biomass on the other, as well as the effects of mass transport due to the water motions and the exogenous variables, water temperature and incident solar radiation. The particulars relevant to the application of such a model to a setting such as this where there exists large differences in concentrations of biomass and nutrients between Saginaw Bay and Lake Huron proper are discussed. The model is shown to agree reasonably well for both regions simultaneously which provides strong evidence that it is a reasonable representation of the situation in the lake and bay.

Background

Lake Huron, the second largest of the Great Lakes and fifth largest lake in the world, has a water surface area of 23,000 square miles.[1] Saginaw Bay is an inland extension of the western shore of Lake Huron projecting southwesterly midway into the southern peninsula of Michigan. It receives drainage from a basin seven times bigger than the bay itself, or over 8,000 square miles.[2]

Major inflows to Lake Huron proper are from the St. Mary's River draining Lake Superior and across the Straits of Mackinac from Lake Michigan. Other tributary flows enter the lake in Georgian Bay and the North Channel from the Canadian basin and along the State of Michigan shoreline on the U.S. side. Outflow is via the St. Clair River.

The Saginaw River is the major tributary to Saginaw Bay and enters the bay at its southwestern end. It receives both municipal and industrial discharges and its total tributary system drains an area of approximately 6,200 square miles.[1] Significant loading to Saginaw Bay results from the input of the Saginaw River. Since the bay is shallow relative to Lake Huron most of the effect of Saginaw River input is felt within the bay itself. The resultant situation, then, is an essentially oligotrophic Lake Huron with eutrophic conditions in Saginaw Bay.

It is this complex problem setting which the model described herein specifically addresses.

Kinetics of Phytoplankton Biomass

Application to other problem settings[3,4] and in particular a detailed exposition and application to Lake Ontario [5,6] provide the background for the discussion below. The basic structure, assumptions, and compilation of relevant coefficients is also available.[7]

The phytoplankton biomass that develops in a body of water depends on the interactions of the transport to which they are subjected and the kinetics of growth, death, and recycling. The structure of the model is shown in Figure 1. Phytoplankton biomass growth kinetics are a function of water temperature, incident-available solar radiation, and nutrient concentrations, specifically inorganic nitrogen and phosphorus. Phytoplankton also endogenously respire and are predated by herbiverous zooplankton which grow as a consequence. They, in turn, are predated by carnivorous zooplankton whose biomass increases as a result. Zooplankton grazing and assimilation rates are a function of temperature and, for the herbiverous zooplankton, the phytoplankton biomass as well. Zooplankton respiration is temperature-dependent. The nutrients, which result from phytoplankton and zooplankton respiration and excretion, recycle from unavailable particulate and soluble organic forms to inorganic forms, ammonia and orthophosphate for nitrogen and phosphorus respectively. The recycle kinetics are temperature-dependent. In addition, they are a linear function of the phytoplankton biomass present. The latter assumption is a modification introduced for the Lake Huron model and is based on the following reasoning: the recycling is either being accomplished by the phytoplankton themselves; they break down the soluble organic material prior to assimilation, or by the bacteria present as a consequence of their metabolizing the detrital material. For the former mechanism phytoplankton biomass dependence is expected. For the latter situation, if the rate is dependent on bacterial biomass, and if phytoplankton primary production is the major source of organic carbon for the bacteria, it is reasonable to suppose that bacterial biomass is proportional to phytoplankton biomass, which results in the same dependence of recycle rate on phytoplankton biomass.

In addition to the kinetics described above, the mass balance equations which comprise the model account for the transport of material between Lake Huron and Saginaw Bay, the inputs into Saginaw Bay from the Saginaw River and other sources, and the loss of phytoplankton and particulate detritus via sedimentation. The magnitude of the rate of regeneration of the nutrients associated with the sedimented material is an issue yet to be resolved.

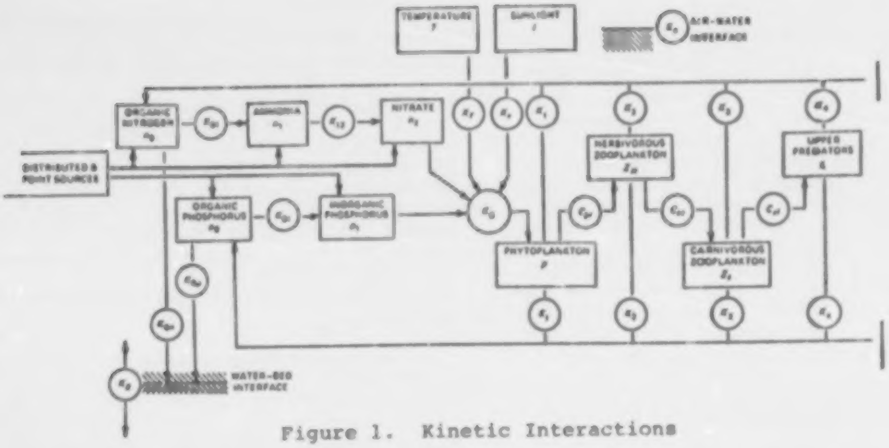
TEMPERATURE
SUNLIGHT
AIR-WATER INTERFACE
ORGANIC NITROGEN
AMMONIA
NITRATE
DISTRIBUTED & POINT SOURCES
ORGANIC PHOSPHORUS
INORGANIC PHOSPHORUS
HERBIVOROUS ZOOPLANKTON
UPPER PREDATORS
PHYTOPLANKTON
CARNIVOROUS ZOOPLANKTON
WATER-BED INTERFACE

Figure 1. Kinetic Interactions

The range of the magnitude of the rate constants for the kinetic terms in the mass balance equations are obtained in the first instance from the literature.[7] The actual values used are obtained by a calibration of the model using a set of observed data which includes observations for every variable computed. For the case of the Saginaw Bay - Lake Huron model, the constants are chosen so that the model reproduces the observed behavior of all variables in both the bay and the lake proper. This is a stringent test of such a model, since nutrient concentrations, primary production rates, phytoplankton and zooplankton biomass differ by an order of magnitude.

Segmentation of the System

The model constructed for Lake Huron is a large spatial scale seasonal time scale model comprising five volumes representing Northern Lake Huron epilimnion and hypolimnion, southern lake epilimnion and hypolimnion and Saginaw Bay. Figure 2 illustrates this model segmentation.

This structure reflects the three characteristic regions of the lake: Saginaw Bay; Southern Lake Huron which is influenced to some degree by the bay due to circulation patterns; and the open waters of the Northern Lake which appears to act as a large receiving body for the inputs from Lakes Michigan and Superior.

The top layer ranges from the surface to a depth of 15 meters which is the depth of stratification. The second layer extends from 15 meters to the lake bottom. The vertical layers are necessary for the incorporation of effects such as biomass sinking with associated nutrient loss from the epilimnion as well as the effects of stratification on nutrient availability.

Data Sources

The verification of a complex eutrophication model requires a large amount of comprehensive, detailed, physical, chemical, and biological data. The credibility of a model is judged, in large measure, by its agreement with observations. Thus a detailed review of available data was made. The historical data for Lake Huron and Saginaw Bay was inadequate in many ways so that a coordinated survey effort was mounted in 1974. The agencies involved were: the Canada Centre for Inland Waters (CCIW), University of Michigan, Great Lakes Research Division (GLRD), and Cranbrook Institute of Science (CIS) with both GLRD and CIS under the direction of the Environmental Protection Agency, Grosse Ile Laboratory. CCIW concentrated in the Northern Lake, GLRD in the Southern Lake, and CIS in Saginaw Bay.

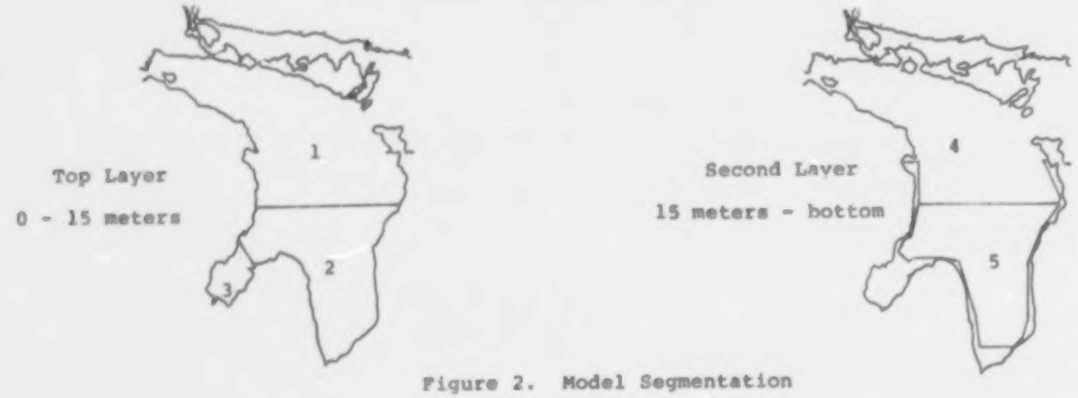
Top Layer
0 - 15 meters
1
2
3
Second Layer
15 meters - bottom
4
5

Figure 2. Model Segmentation

The verification data base which resulted from aggregation of these sources is quite large. Altogether, a total of 35 cruises and about 225 individual sampling stations measured data over a range of depths. The processing of these data for use in model verification requires that means and standard deviations for all stations of each survey within a segment for each cruise be computed. The values for each survey are then overplotted and the result is a set of data for each model segment for all parameters to be verified. The utility of this comprehensive data set cannot be over-emphasized since the historical data prior to these surveys were not adequate for the verification of a lake model of the type presented herein.

Transportation Structure and Verification

The major external influences on Saginaw Bay are the incoming flow of the Saginaw River and a circulating flow from Lake Huron which enters along the northwestern shore and exits along the southeastern shore. The flow has been characterized by several investigators [8,9,10] all of whom have postulated this west to east circulatory flow in Saginaw Bay at least under one generalized type of wind pattern. This Saginaw Bay - main lake flow exchange is incorporated into the model. One of the aims of the transport verification is to estimate its magnitude, since it determines the flushing rate of the bay.

Another feature of the model transport structure is a north to south main lake circulatory flow. Values used are consistent with observed surface velocities, although no strong gradients exist, making it difficult to verify.

The other major aim of the transport verification exercise is to estimate the magnitude of vertical mixing between northern and southern main lake epilimnion and hypolimnion. This is vital to a vertically structured model since it determines the degree of nutrient availability in the open lake epilimnion during stratification.

The verification procedure for transport involves calculating the distribution of a suitable tracer and comparing it to observations. In Saginaw Bay, the horizontal transport regime was verified using the large gradients which exist between the bay and the main lake for temperature, chlorides, and total phosphorus. In the main lake the vertical transport was verified using vertical temperature gradients. Figure 3 shows the observed versus computed profiles for temperature and total phosphorus in the Saginaw Bay model segment and for temperature in the main lake epilimnion and hypolimnion segments. The agreement achieved indicates that the Saginaw Bay transport and the vertical exchange rates are consistent with observation.

Estimates of Nutrient Inputs

Having verified a transport regime and incorporated this into a phytoplankton modeling framework, the only remaining exogenous variables to be specified are the waste load inputs for the parameters to be modelled.

Recently, much new data for Lake Huron waste loading has been made available.[11,12] This comprehensive data base includes Saginaw River loading as well as municipal and industrial inputs for both the Province of Ontario and the State of Michigan, tributary inputs for these same sources including estimates of load contributed by ungaged drainage basins, atmospheric inputs and inputs from the St. Mary's River and the Straits of Mackinac.

Utilizing the best available information, these loads were structured for input to the model. Some significant results of this information are that inputs to Saginaw Bay of approximately 7,000 lbs total phosphorus/day make up about one third of total phosphorus input to the entire lake, that atmospheric sources contribute a significant portion of the total nitrogen (31%), and that most of the impact of Province of Ontario tributary loadings to North Channel and Georgian Bay are felt within those localized areas and do not have a great impact on Lake Huron proper. This formulation is used for model verifications.

Phytoplankton Biomass Model Verification

Figure 4 illustrates computed versus observed profiles for phytoplankton chlorophyll, zooplankton, ammonia and reactive phosphorus, for the Saginaw Bay and northern and southern main lake epilimnion model segments. Other parameters which were equally well verified were total phosphorus, nitrate, and primary productivity.

Phytoplankton chlorophyll in the northern lake epilimnion segment increases during the spring to an early summer maximum limited by available phosphorus. Herbivorous zooplankton grazing then lowers the concentration substantially which then recover as carnivorous zooplankton prey on the herbivors. The secondary recovery utilizes phosphorus provided by the recycle mechanisms. The spring increase of phytoplankton chlorophyll is more pronounced in the southern lake epilimnion segment. Zooplankton predation again causes a decrease with a secondary bloom occurring in the fall. Nutrient patterns are similar to the northern lake epilimnion. Total zooplankton biomass is both calculated and observed to remain substantial throughout the fall months.

It is important to note the order of magnitude difference in concentrations of phytoplankton biomass and nutrients for the Saginaw Bay model segment versus the northern and southern epilimnion model segments. Agreement between calculations and observations indicates that the model is capable of reproducing behavior in both situations. It should be emphasized that the kinetic constants used are the same for both the main lake and the bay.

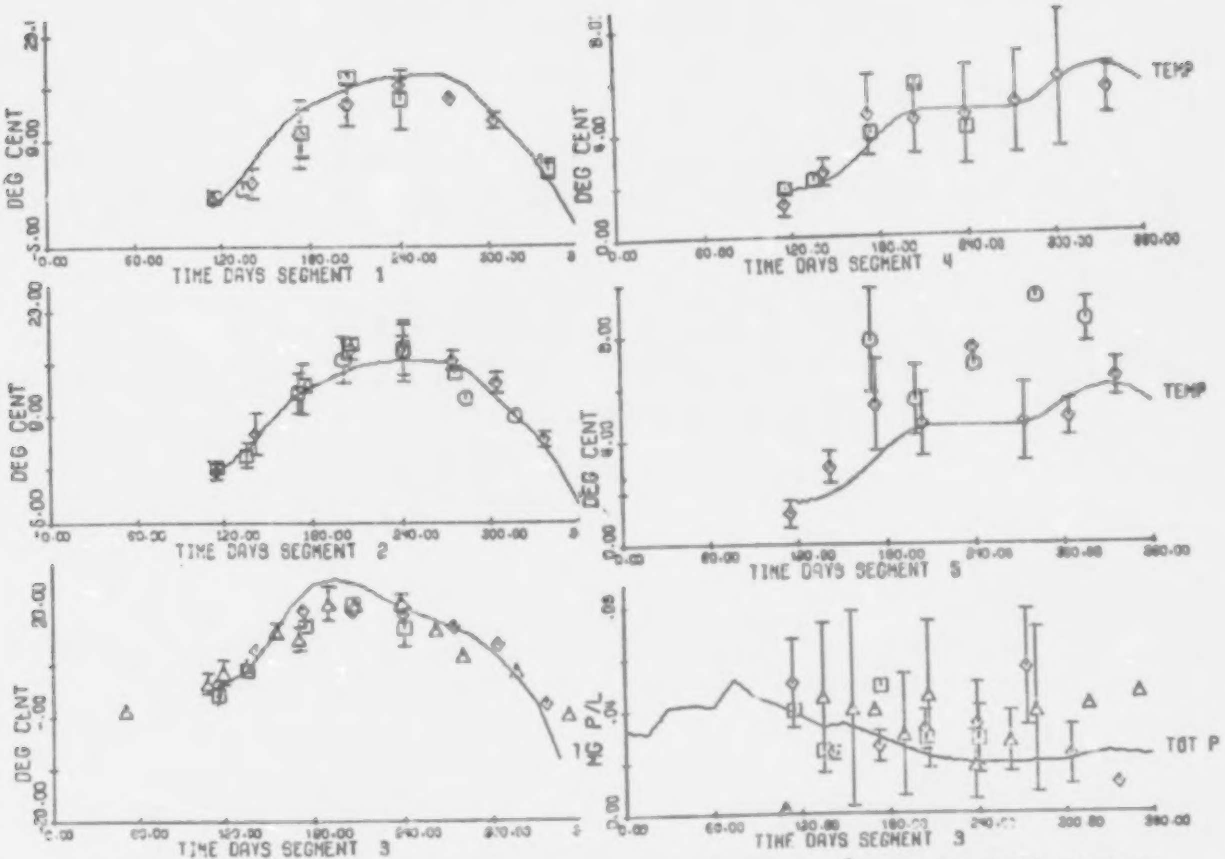

Figure 3. Computed Versus Observed Profiles for Temperature (^{o}C) in All Model Segments and Total Phosphorus in the Saginaw Bay Model Segment

Conclusions

It is common to require as a criterion for verification of a model that it reproduces observed phenomena over a range of environmental conditions. It is especially useful if the conditions cover the region for which model projections are desired. Althougn this is seldom possible, the Saginaw Bay - Lake Huron model does reproduce observations which vary over a wide range of nutrient concentrations. Hence it appears reasonable to claim that the model is verified at least to that extent. The significance, then, of this verified model is that it becomes a useful planning tool to estimate the effects of nutrient reduction policies. These policies will tend to lower the concentrations in Saginaw Bay and thereby bring values closer to Lake Huron values for which the model is also verified.

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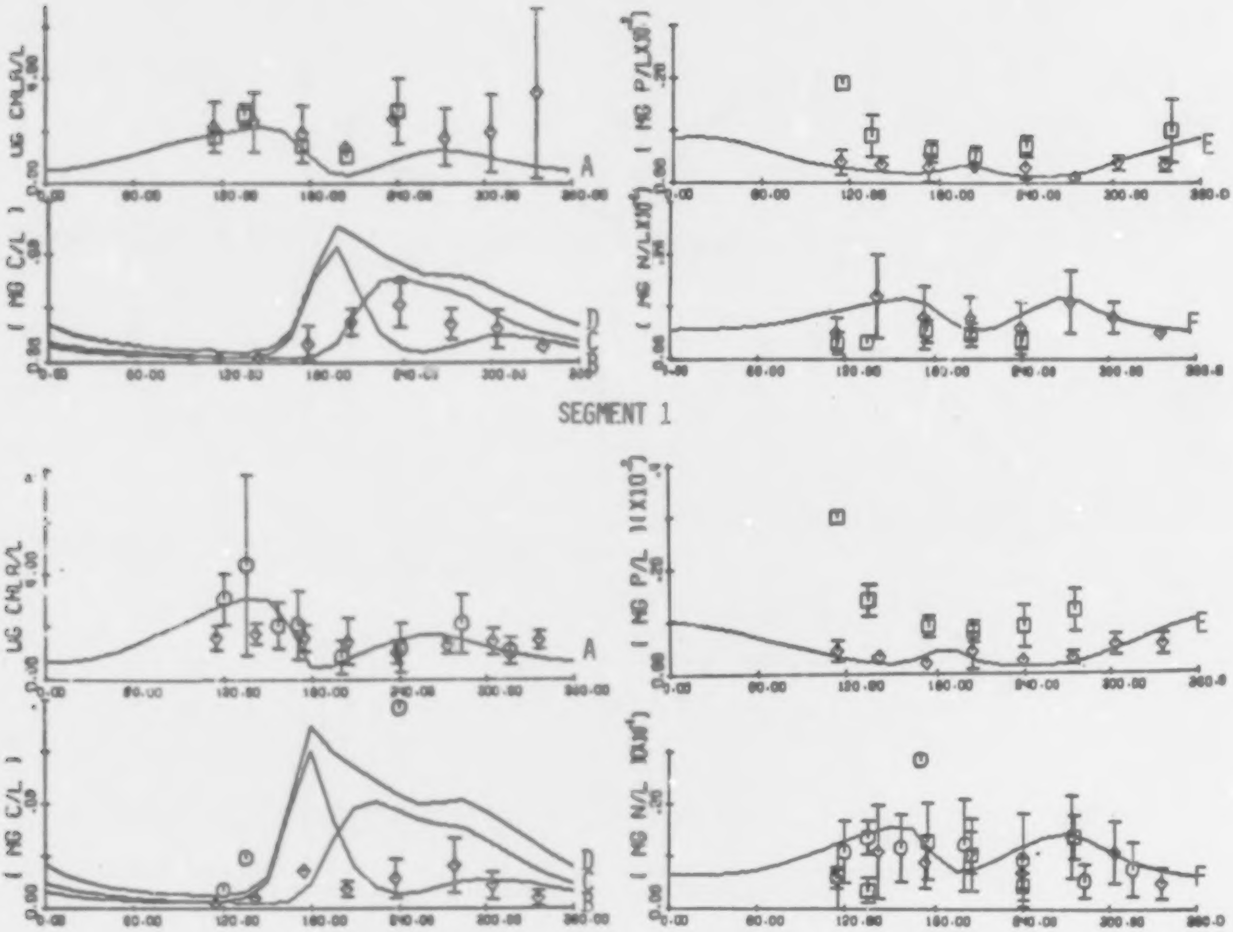

Figure 4. Computed versus observed profiles for phytoplankton chlorophyll (A); herbivorous (B), carnivorous (C), and total (D) zooplankton; ammonia nitrogen (E); soluble reactive phosphorus (F) in northern lake epilimnion (segment 1), southern lake epilimnion (segment 2) and Saginaw Bay (segment 3) model segments.

COMPARISON OF PROCESSES DETERMINING THE FATE OF MERCURY IN AQUATIC SYSTEMS

Lassiter, R.R., Malanchuk, J.L., Baughman, G.L.
Environmental Research Laboratory
Athens, Georgia

Summary

An analysis of factors affecting the fate of mercury in aquatic systems is made using a mathematical model. Three forms of mercury (mercuric, elemental, and methyl) are represented. All forms are considered to be present in both the water and sediment portions of the system. Processes influencing the behavior of mercury forms are assumed to be oxidation, reduction, methylation, demethylation, sorption, sediment/water exchange, volatilization, and longitudinal transport. Environmental factors of importance are pH, concentration of suspended particulates, depth of water, and depth of sediment. Three dimensional graphs (concentration vs. time and distance) are used to portray the temporal behavior of the mercury forms along a stretch of slowly moving stream. Mercuric mercury flows through the reach, partitioning into the sediment as it flows. The spatio-temporal pattern of methyl and elemental forms in both water and sediment is controlled largely by the mercuric mercury sorbed to the sediments. This effect and the sensitivity of all the forms to a range of values used for the sediment/water partition coefficient for mercuric ion, lead to the conclusion that sorption is the single most important factor influencing the behavior of mercury in aquatic systems. There is a slow loss of total mercury to the system by volatilization. Predicting the concentrations of mercuric mercury species in a system accounts for most of the total mercury. However, the model, directed toward environmental pollution predictions, must also account for the fate of low-level but hazardous forms such as methyl mercury.

Introduction

The fate of mercury in environmental systems results from the concurrent functioning of many processes. Some of these processes respond in complex ways to several environmental factors. For example, one pathway of oxidation of elemental mercury is a function of the oxygen concentration and hydrogen ion concentration; the extent of sorption of mercuric ion is a function of the concentration and nature of the particulate material, the hydrogen ion concentration, and other factors.

Simultaneous (parallel) processes are competitive, yet any one of them may operate in a chain of serial processes, e.g., sorption of mercuric ion *could* act as the concentrator for microbially mediated methylation. The web of interconnected serial and parallel processes forms the biogeochemical cycle of mercury. A necessary condition for predicting the fate of mercury is to have a basic understanding of its biogeochemistry. That condition, however, is not sufficient to permit one to predict its fate, because its biogeochemistry is complex and resources are finite. Thus predicting the fate of mercury becomes an exercise in judicious selection of the chemical forms to consider, the important processes that link these forms, and the resources to use for making the predictions.

Because of the complexities introduced by environmental variables driving these processes, and by the multiplicity of these processes occurring serially and in parallel, a computer model was the means chosen for making the prediction. The forms selected and the processes linking these forms into a biogeochemical cycle were chosen to ultimately permit prediction of methyl mercury and its biological consequences. Before attempting the detailed predictions for methyl mercury, the biogeochemistry linking it and the other two forms, mercuric and elemental mercury, needs to be satisfactorily represented in the model. The biogeochemical cycle linking these forms of mercury in a water/sediment system is represented in Figure 1.

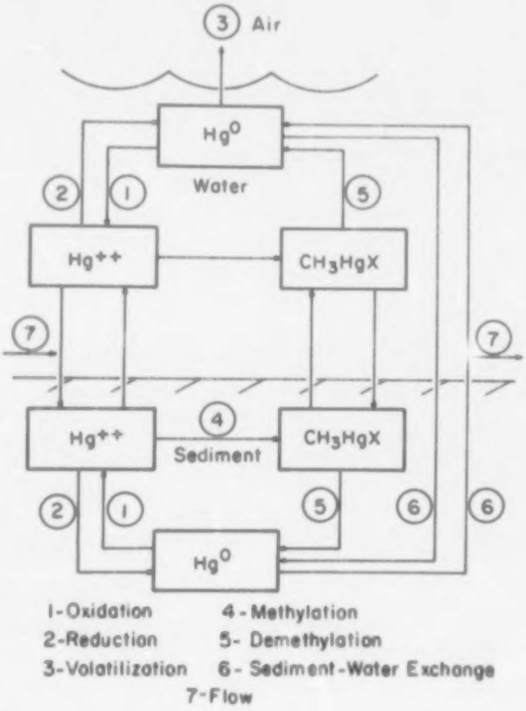

Figure 1. Schematic Representation of the Components, Transformations, Exchanges and Transport Pathways Represented in the Model.

One process, sorption, is not indicated explicitly in Figure 1. However, sorption is represented in the model by partitioning mercuric and methyl mercury into sorbed and dissolved fractions.

Model Description

A set of differential equations is used to describe the dynamics of the forms of mercury in the system. In Figure 2 a set of equations for a system without hydrodynamics is given, using mnemonic abbreviations for the term descriptions.

$$\frac{d[Hg(+2)]_w}{dt} = \text{oxid} - \text{swx} - \text{red} - \text{meth}$$

$$\frac{d[CH_3HgX]_w}{dt} = \text{meth} - \text{swx} - \text{demeth}$$

$$\frac{d[Hg^{\circ}]_w}{dt} = \text{red} + \text{demeth} - \text{swx} - \text{oxid} - \text{volat}$$

$$\frac{d[Hg(+2)]_s}{dt} = \text{oxid} + \text{swx} - \text{red} - \text{meth}$$

$$\frac{d[CH_3HgX]_s}{dt} = \text{meth} + \text{swx} - \text{demeth}$$

$$\frac{d[Hg^{\circ}]_s}{dt} = \text{red} + \text{demeth} + \text{swx} - \text{oxid}$$

Figure 2. Differential Equations Indicating Source/Sink Terms.

swx = sed/water exchange
meth = methylation
volat = volatilization
demeth = demethylation
oxid = oxidation
red = reduction

The aquatic system described by the model consists of a body of moving water in contact with the atmosphere and underlying sediments. The hydrodynamics of the moving water is represented by advection and dispersion terms in one dimension. Each equation is of the form

$$\frac{\partial\,[Hg]}{\partial t} = \frac{D\,\partial^2 [Hg]}{\partial x^2} - \frac{V\,\partial\,[Hg]}{\partial x} + S([Hg])$$

in which Hg represents any one of the forms mentioned above and listed in Figure 2, the first term on the right represents dispersion, the second advection, and the third a set of terms from the appropriate equation of Figure 2, and which represent sources and sinks. The source-sink terms, S, are written as functions of environmental descriptors, e.g., pH, concentration of suspended particulate material, or depth of sediment and water. Although a great deal is known about the chemistry of mercury, none of the source or sink terms can be written without conjecture. Nevertheless, an attempt was made to structure each term to reflect as much as is understood about the chemistry of the process.

An example from the mercury model will illustrate some of the uncertainties accompanying the writing of source or sink terms. Oxidation and reduction of elemental mercury and mercuric ion, respectively, is described by the following equilibrium expression (Parks, G.A., pers. comm.)

$$\frac{[Hg^{0}]\ [H^{+}]^{2} PO_2^{\frac{1}{2}}}{[Hg^{2+}]} = 10^{-19.6}$$

However, observations from several types of experiments show that the reactions do not proceed rapidly to completion, i.e., solutions containing mercuric ion continue to produce elemental mercury for days (1,2,3). Because of these observations the reactions are better represented by rate terms rather than by algebraic equilibrium expressions. Equilibrium expressions do not necessarily reflect mechanisms, and rate expressions cannot properly be obtained from them. In spite of this fact, the following reactions, given by Parks (4), were used to represent oxidation and reduction pathways:

$$Hg^{2+} + H_2O \underset{k_o}{\overset{k_r}{\rightleftharpoons}} Hg^{0} + 2H^{+} + \tfrac{1}{2}O_2$$

The term for oxidation was taken to be

$$k_0\ [Hg^{0}]\ [H^{+}]^{2}\ [O_2]^{\frac{1}{2}}$$

and reduction was

$$k_r\ [Hg^{2+}].$$

For the environment reduction cannot be as simply represented as this term. It is complicated in most natural waters by the presence of suspended particulate material which is probably encased by a layer of organic material (5). Mercuric ion complexes strongly (6) with sulfhydryl-containing compounds and is expected to bind strongly to suspended particulates. The question facing the modeler is whether reduction of mercuric ion bound to particulates can be represented by a simple proportion as assumed for the dissolved fraction. If not, the bound mercuric ion concentration must be computed. The following equations are used as an approximation for computing the bound mercuric ion, also taking into account hydrolysis.

$$Hg^{2+} + H_2O \rightleftharpoons HgOH^+ + H^+$$

$$HgOH^+ + H_2O \rightleftharpoons Hg(OH)_2 + H^+$$

$$Hg^{2+} + \wp \rightleftharpoons Hg + 2H^+$$

Here, $\wp$, is a symbol for suspended particles treated as though they are a dissolved constituent. The three equilibria are

$$\frac{[HgOH^+]\ [H^+]}{[Hg^{2+}]} = K_1$$

$$\frac{[Hg(OH_2)]\ [H^+]}{[HgOH^+]} = K_2$$

$$\frac{[Hg\wp]\ [H^+]^2}{[Hg^{2+}]\ [\wp]} = K_p$$

Assuming that $[Hg^{2+}] << [\wp]$ and is so low that the reactions do not affect $[H^+]$, the set of equations consists of four unknowns $[Hg^{2+}]$, $[HgOH^+]$, $[Hg(OH)_2]$, $[Hg\wp]$. A mass balance equation for Hg_T^{2+} provides the other information necessary for solution:

$$[Hg_T^{2+}] = [Hg^{2+}] + [HgOH^+] + [Hg(OH)_2] + [Hg\wp]$$

The bound fraction, β, is

$$\beta = \frac{K_p[\wp]}{[H^+]^2 + K_1\ [H^+] + K_2K_1 + K_p[\wp]}$$

and the free mercuric ion fraction, δ, is

$$\delta = \left[1 + \frac{K_1}{[H^+]} + \frac{K_2K_1 + K_p\ [\wp]}{[H^+]^2}\right]^{-1}$$

Depending upon whether reduction of only free mercuric ion or of both bound and free can be described by the constant proportion, the reduction term is either

$$k_r\ \delta\ [Hg_T^{2+}]$$

or

$$k_r\ (\beta + \delta)\ [Hg_T^{2+}].$$

Each term in the model was subject to similar uncertainties. The question of how to express accepted chemical, biochemical or other equations in the context of a complex natural system is the basic difficulty facing the "environmental modeler".

Results and Discussion

Figures 3-8 show a pulse input of mercuric ion to the system and its fate in the system, i.e, its transformation to other forms, its transport to the sediment, and its loss from the system. The simulated time is 20 days. Mercuric mercury is introduced and quickly flows through the system (Figure 3) leaving mercuric mercury bound to the sediments (Figure 4) and leaving elemental and methyl mercury transformation products (Figures 5-8).

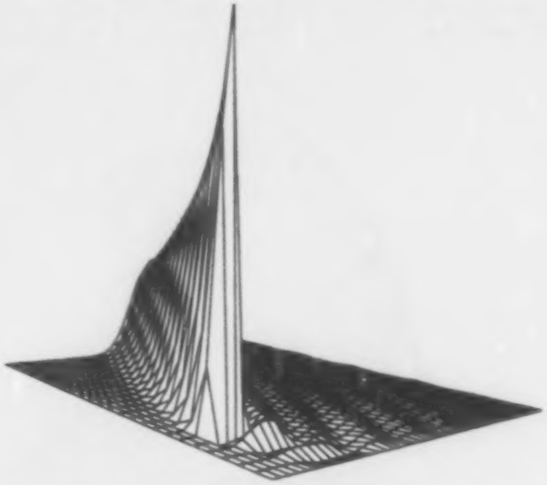

Figure 3. Concentration of Mercuric Mercury in Water Versus Time (Right Axis, 20 Days) and Distance (Left Axis, 1 km).

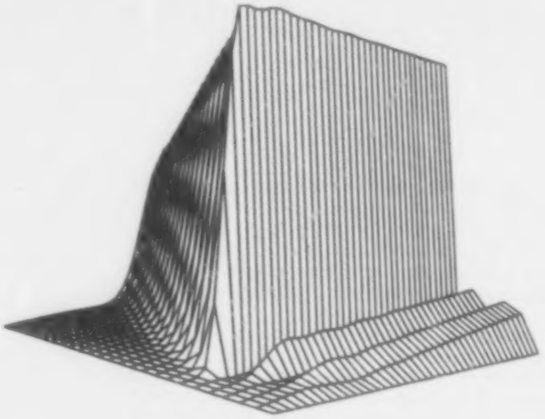

Figure 4. Concentration of Mercuric Mercury in Sediment Versus Time (right Axis, 20 Days) and Distance (Left Axis, 1 km).

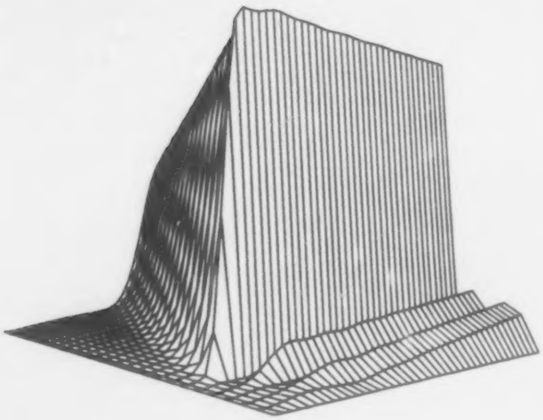

Figure 5. Concentration of Elemental Mercury in Water Versus Time (Right Axis, 20 Days) and Distance (Left Axis, 1 km).

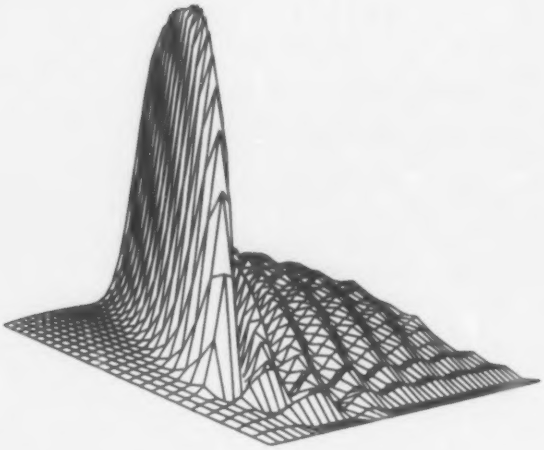

Figure 7. Concentration of Methyl Mercury in Water Versus Time (Right Axis, 20 Days) and Distance (Left Axis, 1 km).

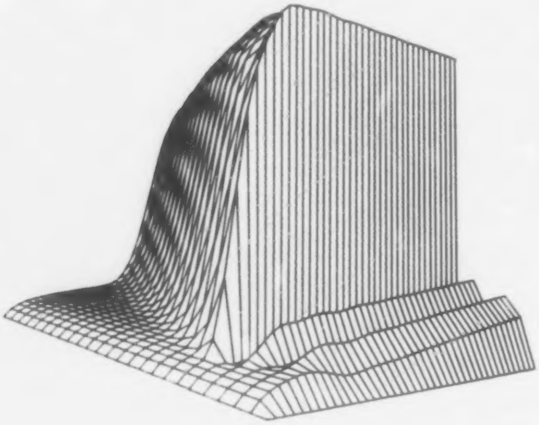

Figure 6. Concentration of Elemental Mercury in Sediment Versus Time (Right Axis, 20 Days) and Distance (Left Axis, 1 km).

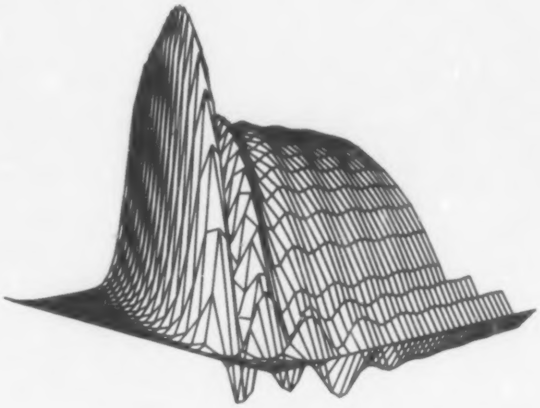

Figure 8. Concentration of Methyl Mercury in Sediment Versus Time (Right Axis, 20 Days) and Distance (Left Axis, 1 km).

Sorption holds mercuric mercury in the sediments so that, unlike the pattern in water, it remains at a point along the stream with loss essentially by transformation only. This gives the graph (Figure 4) its solid appearance relative to that of Figure 3.

In the sediments there is continual transformation of mercuric mercury to the elemental and methyl forms. Graphs of these forms (Figures 5-7) more or less resemble that of mercuric mercury (Figure 4). It is apparent from these figures that sorption is a major controlling factor of the temporal behavior of mercury in aquatic systems.

Only two permanent losses are represented, outflow and volatilization. The effect of outflow is shown in in Figure 3. The effect of volatilization can be visualized by observing that all the slopes of the concentrations with time are negative. These negative slopes result from volatilization of elemental mercury from the water and from recycling of the forms to mercuric with subsequent outflow. Another loss, not explicitly considered, which may be nearly permanent is conversion to mercuric sulfide. However, it can be considered to be implicitly contained in the partition coefficient.

In evaluating the importance of sorption, the partition coefficient for binding of mercuric ion to solids, K_p, was varied over five orders of magnitude, and the behavior of the forms of mercury was observed. Figures 9 and 10 show the behavior of methyl mercury as a result of varying degrees of sorption of mercuric mercury. Methyl mercury concentration was higher in the sediments for smaller values of K_p (Figure 9), whereas the opposite is true of water (Figure 10).

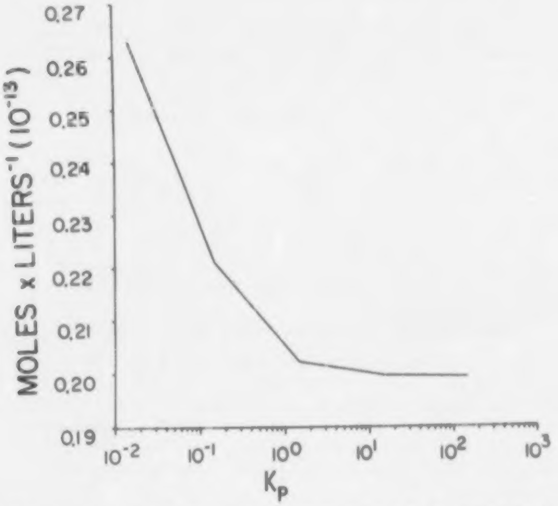

Figure 9. CH_3HGX IN SEDIMENT AS A FUNCTION OF K_p

The bulk of total mercury in a system is undoubtedly some form of mercuric mercury. The elemental form has rarely, if ever, been measured in an environmental sample, and methyl mercury is seldom measured in water samples (7,8). One could delete both elemental and methyl mercury from the model and still account for an overridingly large portion of the total mercury. But elemental mercury is important to the ultimate fate of mercury. It is formed at different rates under differing conditions, and is the only loss from total water systems. Methyl mercury, a minute portion is important because of its health and ecological implications. In general, predicting the fate of a pollutant will consist of predicting the fate of the bulk, *so that the fate of small but hazardous portions can be predicted.*

Conclusions

Using a skeletal model of the environmental chemistry of mercury a few processes emerge as dominant in its fate. Sorption is the most prominent feature in the temporal behavior of mercury. It affects the pattern of loss of mercury from the system by both outflow and volatilization. Predicting the fate of mercury involves not only predicting the fate of the major portion, but also predicting the fate of minute fractions whose health and ecological effects make them important.

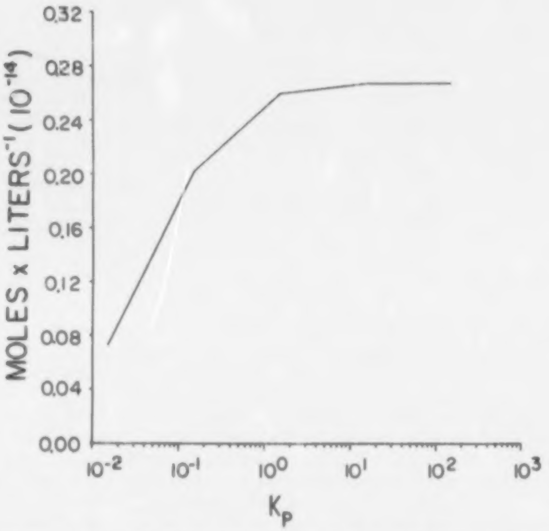

Figure 10. CH_3HGX IN WATER AS A FUNCTION OF K_p

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ASPECTS OF MATHEMATICAL MODELS AND MICROCOSM RESEARCH

James W. Haefner
Department of Wildlife Science
Utah State University
Logan, Utah 84322

James W. Gillett
Environmental Protection Agency
200 SW 35th Street
Corvallis, Oregon 97330

ABSTRACT

Some features of the conceptual structure of a potential mathematical model are presented to illustrate the important role mathematical models can and should play in future microcosm research. Mathematical models can help microcosms achieve their goals of screening exogenous substances, understanding the fate and effects of exogenous substances, and designing suitable management strategies. The conceptual structure reported here emphasizes the role of biotic components in controlling pesticide flows.

INTRODUCTION

As the experimental manipulation of microcosms becomes an increasingly important tool for both pure research and management purposes, it is necessary that the role of mathematical models be clearly delineated. It is our position that mathematical models are extremely useful for research programs embodying microcosm studies. We hope, in this paper, to document this position by showing how the conceptual structure of a potential mathematical model can influence the measurements and experiments of a terrestrial microcosm. The mathematical model itself is still in early stages of forumulation.

A. The Terrestrial Microcosm

Since 1974 the Corvallis Environmental Research Laboratory has been developing and testing a terrestrial laboratory microcosm system for screening the disposition and effects of pesticides. This system was derived from the work of Metcalf et al.[8-2], and from a conceptual model of pesticide fate (Gillett et al., 1974[6]). The basic objective of the program is to develop a tool for screening potentially adverse environmental behavior of pesticides by assessing the fate of radio-labeled chemicals and quantifying observable effects associated with the introduction of the chemical into the system. A secondary objective is to correlate these dispositions and effects with the physical properties of the chemicals and environmental components and thus synthesize an understanding of the relationships of classes of compounds to ecological effects. It should be apparent that, whereas pesticides are discussed in relation to the studies, one could apply this approach to any potentially hazardous or toxic substance.

The details of this system have been presented elsewhere.[5] It is comprised of (a) a Terrestrial Microcosm Chamber (TMC) and associated biota and support systems; (b) an operational format or protocol; and (c) an analytical scheme for determining the distribution and identification of ^{14}C-residues. The TMC is a 101 x 75 cm glass box with plastic lid enclosing about 40 cm of head space over 20 cm of an artifical soil containing endemic micro-flora and fauna. The unit is semi-closed, in that it is open to energy (heat and radiation supplied by overhead fluorescent and incandescent lamps), while purified air and water are circulated through the TMC and exit to sampling systems (but can be arranged to be closed or recirculating).

Normal operation includes addition of certain terrestrial macrofauna (nematodes, earthworms, soil insect larvae) prior to planting selected crops and weeds (alfalfa, rye grass, corn, soybean). Subsequently higher organisms are added after plant growth has reached the desired level (Collembola, crickets, pillbugs, snails and then gravid vole -- *Microtus canicaudus*).

Experimentation and sampling in the chambers involves the application and monitoring of ^{14}C-labeled pesticides. Variations in these experiments can be achieved by altering the biotic constituents (especially the plant species and planting pattern), the abiotic operating parameters, and the chemical (nature, formulation, quantities, timing, and mode of application).

Monitoring during an experiment includes periodic measurements of the pesticide and its degradation products in the water, air, at specified soil depths, and in selected plant species. Soil moisture and temperature are monitored. The amount of pesticide adsorbed onto the inside surfaces of the box can also be measured frequently. At the end of an experiment (6-8 weeks) the vertebrates are sacrificed to determine the pesticide levels in their tissues. Appropriate concomitant controls are utilized.

B. Model Objectives

The primary objective of the model of the microcosm is to determine the dynamic behavior of ^{14}C-isotope residues when the radioactive label is attached to specified classes of chemicals that are physically applied to the microcosm in known amounts and by known methods. The model is to be constructed so as to permit a mass balance analysis of the residues as they are distributed between diverse components and compartments of that ecosystem. To accomplish this the mathematical model must provide under the biotic and abiotic conditions prevailing at the time of the experiment a dynamic description of:

(1) the amounts of pesticide (exemplified by "dieldrin" and "parathion") and its products that are incorporated into plant and animal tissues, bound to biotic components, or removed from the microcosm via water and air;

(2) the amounts of pesticide transformed into major derivative by-products (metabolites, conjugates, or bound residues);

(3) the effects of the pesticide and by-products on the feeding, growth, and reproductive behavior of the organisms in the microcosm;

(4) the effects of the feeding, defecation, movement and related behavior of the organisms in the microcosm on the disposition and movement of the pesticide;

(5) the amount of CO_2 and organic carbon present in (a) the living tissue of the organisms, (b) non-living particulates, and (c) both the atmospheric and water portions of the microcosm; and

(6) the effects of abiotic conditions (e.g., temperature, pH, and soil moisture) on the processes governing the movement and transformation of the pesticide.

MODELING APPROACH

The primary concern of this model is the movement of a pesticide among the components of a terrestrial microcosm. These components include both biotic and abiotic elements and a model must incorporate both. This is accomplished in this modeling approach by explicitly modeling the role that biota play in regulating pesticide movement.

The concept of biotic control of abiotic processes can be given a very simple structural description, illustrated in Figure 1. The Pesticide Transport Process (PTP) is a system that receives inputs from external sources and from the Biotic Control Processes (BCP). In addition, PTP delivers outputs to external sinks and to BCP. PTP also possesses internal pathways and feedbacks that are symbolized by the curved, self-directed arrow. The BCP component is structured in much the same way; it has external sources and sinks, internal feedbacks, and a coupling with PTP. In later discussion, the coupling of PTP and BCP will be referred to as the "control system."

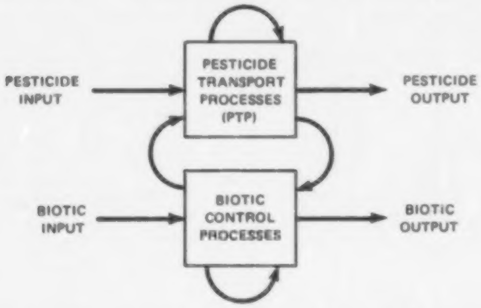

Figure 1. Diagrammatic representation of the control system. Shown are its two basic components: pesticide transport and biological control.

The control system approach to modeling pesticide disposition has several advantages that are important enough to note. First, this approach is more realistic since it specifically includes the mutual actions and effects of organisms and pesticides. At the same time, by uncoupling pesticides and biological flows except for control effects, the model structure takes cognizance of the minor effect the biota have on the mass flow of pesticides in natural or constructed ecosystems. Second, the control system approach permits simulation experimentation on the counter-intuitive effects that pesticides have on a particular biota (including economically important crops) through actions on other pathways or components in the food web. Third, the uncoupling aspect of the control system is important because the dimensions of state variables describing pesticide disposition (molar equivalents of ^{14}C) differ from the contents of state variables describing the biota (grams of C). Models with consistent equations require state variables with consistent units.

A. Pesticide Transport Processes

Figure 2 provides more detail of the control system approach. For the purpose of the PTP the microcosm is composed of four layers: an above-ground subsystem, soil layer I, soil layer II, and soil layer III (the number of layers is not fixed and can easily be either increased or decreased). Each layer is composed of a "center" and an "edge". Within the three soil layers are two different classes of soil types: Isolated (I) and Contiguous (C). Isolated soil is soil that has no connection with the atmosphere by means of its interstitial connections. Contiguous soil has a direct, if not straight, connection with the atmosphere. It is assumed, further, that the vapor phase in contact with contiguous soil is in equilibrium with the above-ground atmosphere, although there may be indirect connections with the atmosphere by means of soil water. This distinction is important in describing volatilization of pesticides from soil particles. Volatization can occur and have an input to the above-ground atmosphere only if the surface of the soil particle is connected, in the gaseous phase, to the above-ground atmosphere. It seems clear, also, that the fraction of isolated soil will increase with increasing depth from the surface and increasing percent soil moisture. This provides a good operation definition of soil layers. The "surface" (soil layer I) can be defined as that set of depth intervals for which the soil possesses, for example, 5% or less isolated soil. One can also define soil layer III to be that set of depth intervals for which the soil possesses 5% or less contiguous soil. Other layers can be defined in a similar way.

The total volume of soil comprising the surface will vary in time. This variation will be caused by the dynamics of such processes as moisture fluctuations, tunneling, and root growth. As a result, for computational purposes the terrarium will be divided up into many thin "layers" each of which can be described by its percent isolation. Since the total amount of pesticide volatizing in any time step will be a function of the total volume of "surface" soil present, it will be necessary to sum the volumes of all layers meeting the criterion for soil layer I.

Within each of these compartments (layers; edge, center; isolated and contiguous) certain processes of pesticide movement and transformation occur. Those that will be discussed in this report (after Gillett et al.,[6]) are movement by mass flow in water, adsorption, volatilization, and transformation. Figure 2 shows the basic control system of biota and pesticide movement plus some detail in the pesticide component. Most pesticide movement in PTP is associated with physical transport by water flow. Within the soil, gravity, diffusion, and capillary action are forces and processes for transferring pesticides dissolved in water. A certain fraction of pesticides volatizes from contiguous soil and may be lost from the system through the exhaust system or may adsorb onto above-ground surfaces. Because of water condensation on the walls and roof some atmospheric pesticide may find its way back to the soil. Within the soil a portion of the pesticide may adsorb more or less severely to soil particles.[1] The water moving through the soil may leach some pesticide to groundwater.

Besides the direct control effects of the BCP on these pesticide processes (described below), there are a number of important abiotic factors that influence their rates: temperature, moisture, pH, and ionic content. These not only directly alter the rates of pesticide movement, but they influence, and are indirectly influenced by, the BCP as well.[1] Thus, the biota have both direct and indirect effects on the PTP.

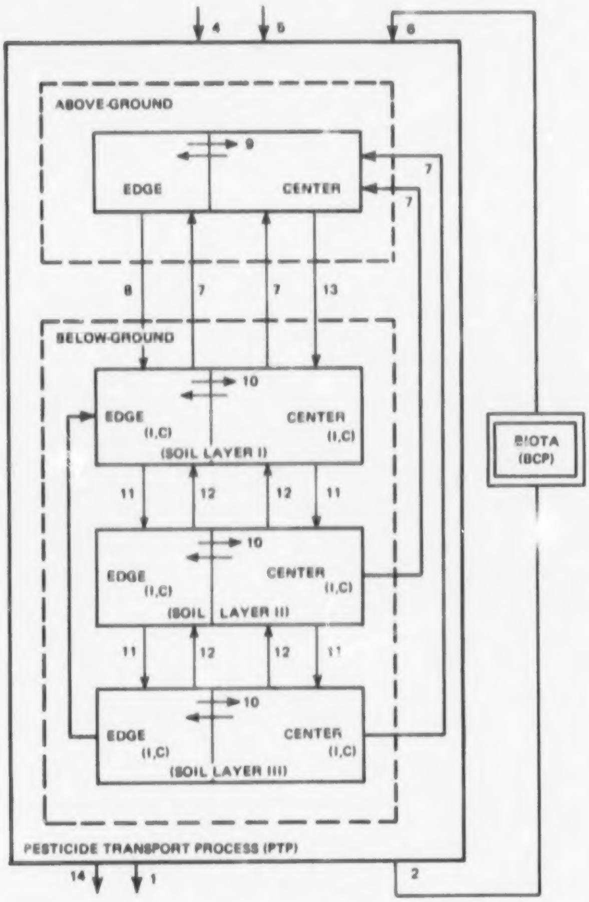
4
5
6
ABOVE-GROUND
9
EDGE
CENTER
7
7
8
7
7
13
BELOW-GROUND
10
EDGE (I,C)
CENTER (I,C)
(SOIL LAYER I)
11
12
12
11
10
EDGE (I,C)
CENTER (I,C)
(SOIL LAYER II)
11
12
12
11
10
EDGE (I,C)
CENTER (I,C)
(SOIL LAYER III)
BIOTA (BCP)
PESTICIDE TRANSPORT PROCESS (PTP)
14
1
2

Figure 2. The processes of pesticide transport in the microcosm. Processes are denoted by number. (1) = loss from atmosphere and unrecycled water, (2) = loss to biota plus effects on Biota, (3) = recycled water, (4) = water input, (5) = pesticide application, (6) = input from Biota plus control by Biota, (7) = volatization from contiguous (C) soil, (8) = runoff from walls and roof, (9) = adsorption and desorption onto walls and roof, (10) = lateral movement in soil, (11) = gravity flow of water and pesticide, (12) = upward diffusion and capillary action, (13) = adsorption onto soil surface, (14) = degradation. Unit of flow within PTP is molar equivalents of ^{14}C.

In addition to physical removal from the microcosm by the air and water evacuation systems a molecule of pesticide may also disappear because of degradation or transformation. This PTP process (via photolysis and hydrolysis) is accelerated by the BCP (via metabolic transformation).

B. Biotic Control Processes

In this section we illustrate the role of the BCP in the control system by describing those portions of the BCP that interact with the PTP as shown in Figure 2. As stated in the model objectives the substance of flow in the BCP is carbon. The general pattern of this flow is shown in Figure 3. The below-ground ecosystem is further elaborated in Figure 4; the "higher trophic levels" compartment is elaborated in Figure 5. These relationships permit us to enunciate some of the mechanisms by which the PTP and BCP interact in this model.

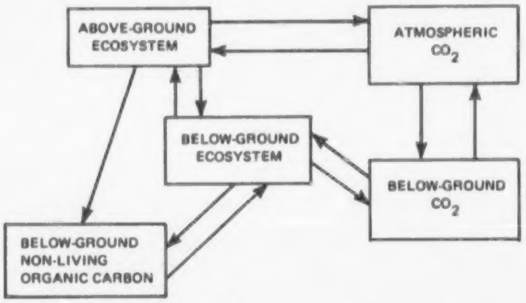
ABOVE-GROUND ECOSYSTEM
ATMOSPHERIC CO_2
BELOW-GROUND ECOSYSTEM
BELOW-GROUND CO_2
BELOW-GROUND NON-LIVING ORGANIC CARBON

Figure 3. The basic structure of the biotic component of the microcosm control system. Unit of flow is carbon.

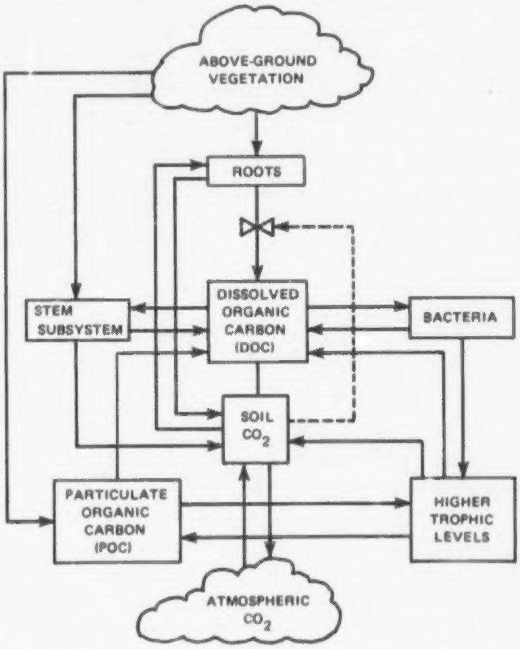
ABOVE-GROUND VEGETATION
ROOTS
STEM SUBSYSTEM
DISSOLVED ORGANIC CARBON (DOC)
BACTERIA
SOIL CO_2
PARTICULATE ORGANIC CARBON (POC)
HIGHER TROPHIC LEVELS
ATMOSPHERIC CO_2

Figure 4. Generalized trophic processes of the below-ground ecosystem. Unit of flow is carbon.

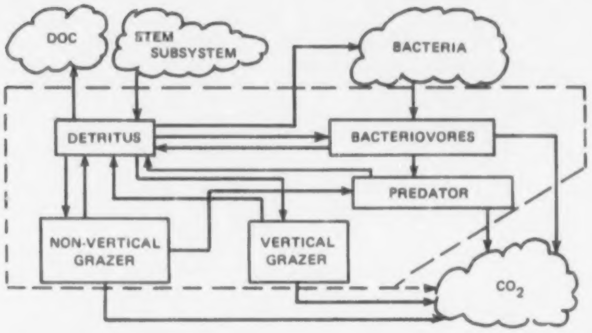

Figure 5. Inter-relations of the higher trophic level subsystem.

An important effect of the biota on the ecosystem is the alteration of the physical structure of the soil. By tunneling, compaction, and root growth the biota alter the effects of gravity, diffusion, and capillary action on patterns of movement of water and therefore, pesticide. Conversely, a major effect of pesticidal toxication on the biota is to alter gross behavior such as "tunneling" (Figure 6). Vertical grazers influence vertical flows between layers directly by their tunneling activity (as represented by the dotted information arrow from "vertical grazers" to "tunneling factor"). The effects of the pesticide can alter this behavior without significantly affecting the amount of carbon contained within a state variable (e.g., "vertical grazer"), as represented by an informational arrow from PTP to the "tunneling factor".

The biota also influence the physical structure of the soil by the production of Particulate Organic Carbon (POC) that has great adsorptive potential. Such particles include solid feces, exoskeletons, root parts from sluffage, and so on. Moreover, organisms that move horizontally alter mechanically the flow rates between the Edge and Center compartments (Figure 6).

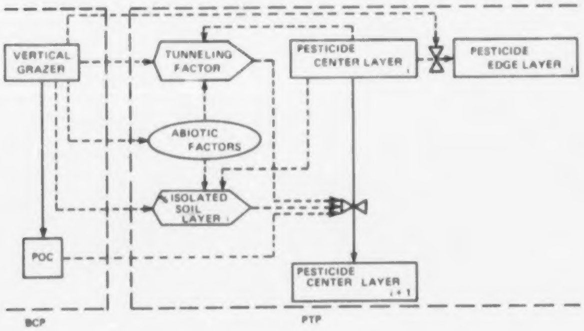

Figure 6. Illustrative interactions between BCP and PTP.

The Dissolved Organic Carbon (DOC) compartment is important in determining carbon fixation. Bacterial metabolism is predominantly internal so that organic material must be in dissolved form to be utilized by bacteria. Because different organic substances (cellulose, hemi-cellulose, lignins, sugars, etc.) have different decomposition rates (Edwards, et al.,[4]; Dickinson and Pugh,[3]) both the quantity and quality of DOC must be considered. Mayberry, et al.,[7] present experimental data which suggests how this can be done efficiently. They have shown that pure strains of bacteria yield 3 gm of cells per equivalent "available electron" in the substrate. An "available electron" is one which is "not involved in a molecular orbit with oxygen" in the structure of the substrate (reference 7). This interesting approach should be pursued, since co-metabolism is the driving force permitting bacterial biotransformation of pesticides.

In these few figures we have indicated some sections of a model designed to study the complex interactions between biotic and abiotic components of microcosms. In what follows we articulate how such models may guide microcosm research.

RELEVANCE OF MODELING TO MICROCOSM RESEARCH

The conceptual structure of this model and the processes of elaboration and documentation that will provide a functional mathematical statement for simulation experimentation are intimately involved in the overall achievement of the several objectives of the microcosm research program, i.e., screening, understanding of ecosystem processes, and development of effective management strategies. Current studies on pesticides in microcosms rely on empirical efforts that need a sound, theoretical basis. Outputs for screening decisions are based on a relatively small number of observations (in comparison to that number which might be used); a successful model would help assuage criticism of those empirical measurements by revealing the necessary and sufficient data points most crucial to the disposition of a given chemical. Further, the integrating process within the model and the requirement of the mathematical model for explicitness should reveal features of the disposition or effects not visible in the empirical approach.

The conceptual model has already enunciated several aspects of the microcosm system that need theoretical or pragmatic definition: the distinction between "edge" and "center", the "isolated" vs "contiguous" soil, the "tunneling factor" and other behavioral variables, and the interaction between pesticides and abiotic factors in their effects on carbon flow in BCP. Explicit hypotheses have suggested particular experiments, and eventually the mathematical model should reach a state where mathematical simulations can be performed. Then parameter sensitivity analysis and other modeling techniques should lead to further improvements in critical analysis of microcosm tests.

Mathematical modeling is also directing microcosm research toward better understanding of the processes of disposition and effect of classes of chemicals. A dynamic, simulation model places emphasis on elucidation of rates of flows and their controls, rather simply on the measurement of state variables. The interaction between the microcosm research program and the Benchmark Chemical Program becomes clearer and more explicit as one considers the need for high quality physical chemical data to parameterize the model processes. As the relationships between the benchmarks and the parameters are better understood, then simplification of process diagnostic analysis should result, especially with the aid of computer model simulation.

Finally, a mathematical model based on the present conceptual structure can also influence management strategies based on microcosm research. Simulation experiments can explore the requisite control characteristics needed to effect a particular pesticide disposition, by indicating the restricted classes of natural ecosystem to which the pesticide might be applied without disrupting the ecosystem or the pesticide disposition goals (i.e., delivery to target for effective time). Alternatively, the model might indicate management action required to counteract adverse disruption of the system or disposition goals when the target area is not in one of the above classes.

CONCLUSIONS

In this paper we have reviewed sections of the conceptual structure of a mathematical model as it pertains to the improvement of microcosm research. We have used this discussion to show how models of microcosms may aid the achievement of the microcosm objectives of screening, understanding, and management strategies. Our emphasis has been complex and subtle interactions between pesticides and the biotic component of terrestrial microcosms. This was formalized by the "control systems" approach which constitutes the core of the conceptual structure. Our recommendations for future microcosm research emphasize investigations of the distinction between soil sectors and their properties, the behavioral effects of pesticides on biotic components of the microcosm, and the interaction of abiotic inputs with pesticide effects.

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AN ECOLOGICAL MODEL FOR THE GREAT LAKES[1]

by

Donald Scavia, Brian J. Eadie, and Andrew Robertson
National Oceanic and Atmospheric Administration
Great Lakes Environmental Research Laboratory
2300 Washtenaw Avenue
Ann Arbor, Michigan 48104

Summary

A one dimensional ecological model, developed and calibrated for Lake Ontario, has been applied to the other Great Lakes to test its generality. The model, physically segmented into two layers, simulates concentrations of phytoplankton, zooplankton, detritus, phosphorus, nitrogen, and total inorganic carbon. Driving the ecological model with physical data from the other Great Lakes results in accurate simulations for the upper lakes after minor recalibration of the kinetics; however, the western and central basins of Lake Erie could not be simulated due primarily to the effects of physical phenomena which are not considered in the model (e.g., sedimentary regeneration of nutrients, resuspension).

The kinetic recalibration involved the adjustment of two coefficients, one representing algal phosphorus requirements (the half-saturation constant for growth on phosphorus) and the other determining the regulation by food of zooplankton growth. The adjustment of these coefficients was based on the theory of competitive succession.

As a result of the verification tests the following conclusions were reached:

(1) For an ecological model to be able to predict ecological changes occurring during eutrophication, it must include at least several compartments in each level of the food chain to allow natural selection to be simulated. In this way "recalibration" will take place automatically as succession and adaptation would in nature.

(2) Further investigations are needed to gain insight into the mechanisms that allow phytoplankton and zooplankton to exist in varying environments. The mechanisms governing the succession and adaptation of species will have to be studied in order to develop mathematical relations that describe these mechanisms.

(3) In some lakes, especially shallow ones, the effects of physical and chemical interactions between sediment and the water column can greatly influence the seasonal dynamics of the lake biota. Models should account for these processes when they are important.

(4) The seasonal effects of allochthonous loads should be included in a eutrophication model for lakes with short residence times.

(5) Once the model discussed in this paper has been parameterized to include coefficients of the individual phytoplankton and zooplankton groups, it should be broad enough for rather general application.

Introduction

There presently exist two broad classes of aquatic models: (1) general, relatively simple models, based on large diverse data bases and usually addressing a single water quality variable[1,2,3] and, (2) more site-specific, complex ecological models, developed for a particular system or system-type and usually simulating many ecologically significant variables[4,5,6,7]. Models of the first group are generally designed to transform simple input into useful output. While these models provide accurate predictions of their respective parameters, they do not address many of the questions pertinent in water resource management. The second category of models attempts to address more specific water quality parameters and processes (i.e., concentrations of phytoplankton groups; seasonal dynamics of the model components; and phosphorus, nitrogen, light, and temperature limitation) but have been indicted as losing their generality during the development of complex process formulations and the evaluation of coefficients[36].

The generality of a model is most critical to its applicability; that is, if a model is very specific, its use beyond simulating historical data is disputable. Very specific models may be useful for testing certain hypotheses, but extrapolations into the future and to other bodies of water are of questionable validity.

The purpose of this paper is to investigate the potential generality of the Lake Ontario ecological model developed by Scavia et al.[4] by applying it to all five of the Lauentian Great Lakes.

Lake Ontario Calibration

This model was developed parameterized, and calibrated for Lake Ontario and has undergone extensive testing for ecological realism[4]. It includes calculations of the concentrations of available phosphorus, dissolved organic nitrogen, ammonia, nitrate, non-living particulate organic carbon, inorganic carbon, four groups of phytoplankton, six groups of zooplankton, and benthic macroinvertebrates. Solution of the equations describing the biological processes is accompanied by calculation of diffusion and sedimentation between three vertical segments, as well as of the concentrations of the components of the carbonate equilibrium system. The ecological model, driven by temperature and diffusion calculated by a physical model based on the work of Sundaram and Rehm[8] and by solar radiation, represents the open-water zone of Lake Ontario.

Certain modifications were made to the existing model to aid in its application to the other lakes. The physical segmentation of the model was reduced from three to two segments: the epilimnion and hypolimnion, and the solar radiation and driving data for the physical model were obtained from climatological studies[9,10,11,12]. Also, the method of numerical integration was changed from a fourth order, variable-step Runge-Kutta-Merson algorithm to a simple, forward step Euler procedure.

None of the alterations seriously affected the results obtained for Lake Ontario. For a complete list of coefficient values and initial conditions for Lake Ontario consult Scavia et al.[4]

Verification: Application to the other Great Lakes

Data for verification were obtained for all the Great Lakes from two sources -- a broad survey of the literature and unpublished measurements[35] made by

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[1] Contribution No. 64 of the Great Lakes Environmental Research Laboratory, NOAA, Ann Arbor, Michigan.

GLERL.

With few exceptions, the available phytoplankton data are reported as chlorophyll or total biomass. For this reason, the values for concentrations of carbon obtained for the four phytoplankton groups in the model have been combined. This total has then been compared to the actual measurements after these were converted to carbon by assuming a carbon to chlorophyll ratio of 50:1 or a fresh weight biomass to carbon ratio of 10:1. Further, the literature values are usually only representative of surface (0-5m) conditions, whereas the model simulates average epilimnetic conditions. This difference is critical during late summer-early fall when simulated epilimnion depths reach over 30 m in most of the Great Lakes. Predictions of average concentration of the phytoplankton in the epilimnion segment will usually underestimate the observed surface (0-5 m) concentrations.

The total zooplankton carbon prediction is the summation of the five epilimnetic zooplankton groups of the model. These five groups do not necessarily represent all of the zooplankton present in the lakes, and the literature generally provides only values for crustacean carbon. Because the predictions and the observed data do not exactly correspond, we are limited to comparing the general dynamics and approximate concentrations of the zooplankton. Data from the 50 m vertical hauls are used for comparison to the average epilimnetic concentrations calculated by the model.

The seasonal nutrient values[35] from the model are average epilimnion concentrations based on the predicted segment thickness, while most of the ranges in the literature are for surface conditions.

The data used for comparisons and to drive the model are limited at this point, and results from the following verification give only an indication of the model's validity for each lake. While caution is urged in interpreting the results, one can consider the potential generality (and limitations) of such a model.

Initial Simulations

The initial verification test consisted of using the coefficients determined by the Lake Ontario calibration and the physical driving data and initial conditions for each new lake or basin. The results of each simulation were then compared to the observed data. The simulations of phytoplankton for the upper lakes (Superior, Huron, and Michigan) resulted in generally lower predictions than corresponding measurements. Also, in all three lakes the predicted zooplankton concentration decreased sharply throughout the year. Lake Erie was considered as three separate lakes: the shallow western, larger central, and deeper eastern basins. The simulations of all three basins failed in a fashion similar to the upper lakes, but additional constraints were also evident and will be discussed later.

In an attempt to explain the poor verification of our model for lakes other than Ontario, we considered the differences in trophic status among the lakes. Differences in nutrient levels are most certainly an important factor in determining the dominant species in the phytoplankton community of a lake. Taking this argument one step further, one can also hypothesize that differences in types and abundance of phytoplankton in lakes will result in shifts in dominance and in intraspecific adaptations within the zooplankton community. Since the original model had been calibrated to the indigenous biota of Lake Ontario, we concluded that, with these coefficient values, accurate predictions would only be possible for lakes with trophic status similar to that of Lake Ontario.

The structure of the model, however, is such that the coefficients describe the state variables on a species-type level whereas the formulations are based on functional relationships and should be consistent for all species within the modeled group. With this in mind one would expect the model could be recalibrated for each new lake.

There are procedures available for efficient curve fitting, and the use of trial-and-error could also lead to recalibrated simulations of the lakes; however, such simulations would not be very interesting or useful, for they would not produce any additional information about the lakes or even the model itself. Instead, we have varied a minimum number of coefficients in an ecologically prescribed manner to determine if simple recalibrations can lead to simulations that agree to a substantial degree with the available data.

The selection of these coefficients was based on two assumptions: (1) the Great Lakes phytoplankton are, for the most part, phosphorus limited, and (2) the relative dominance of specific phytoplankton and zooplankton groups has been determined by the specific environments of the lakes. The model equations involving these two assumptions are the nutrient-regulated growth equation for phytoplankton and the food-dependent grazing equation for zooplankton. The coefficients critical to these mechanisms are the half saturation constants of phytoplankton growth on phosphorus (XKP) and of zooplankton grazing on total food (XKG). A complete description of these constructs can be found elsewhere[4].

Low nutrient levels in Lake Superior probably have favored the dominance of algal species with the ability to grow successfully at these concentrations. This is represented mathematically by a low half-saturation constant. XKP has generally been reported between 1 and 10 μgP/l[13,14,15], so we used 1.0 μgP/l for oligotrophic Lake Superior. The constants for the other lakes were selected (Table 1) following the trophic schemes suggested for the Great Lakes by Vollenweider et al.[16] and Dobson et al.[17]

Table 1. Predicted trophic status variables and recalibration coefficients.

Parameter	Superior	Huron	Michigan	E. Erie	C. Erie	Ontario	W. Erie	Comment
Maximum Phytoplankton	.05	.12	.15	.28	.31	.56	.83	mgC/l
Sedimentation	5.6	7.6	8.3	11.6	10.3	21.6	8.7	$gC/m^2/yr$
	.04	.13	.10	.36	.43	.26	1.09	$gC/m^3/yr$
Maximum Production	110	438	411	775	706	1648	1026	$mgC/m^2/day$
Available Phosphorus	0.1	0.2	0.3	0.6	0.7	0.6	0.5	minimum
	1.0	3.0	4.0	8.0	9.0	15.	25.	maximum
Inorganic Nitrogen	.26	.21	.24	.09	.05	.06	.23	minimum
	.29	.26	.32	.19	.16	.27	.64	maximum
XKP	1.0	2.0	5.0	6.0	8.0	9.0	10.0	μgP/l
XKG	.02	.04	.08	.16	.16	.16	.16	mgC/l

The coefficient relating zooplankton grazing to food concentration (XKG) has not been as thoroughly studied as XKP. Data from Richman[18] imply a value of 1.3×10^4 cells/ml or, in terms of carbon, 0.16 mgC/l for this constant. This value worked rather well in the Lake Ontario calibration and is therefore considered to be in the higher end of the range for XKG. The nutrient-poor waters of Lake Superior support a sparse food supply for the zooplankters, and species adapted to such conditions have most likely been favored. Mathematically this would be represented by a lower value for XKG. The lower extreme of the range for XKG was set at 0.02 mgC/l based on relative phytoplankton concentrations in Lake Superior and Ontario[17,19], and the values for the remaining lakes were determined in the same way as those for XKP (Table 1).

With only these two changes, the model was rerun for the various lakes. Selected aspects of the results are compared to reported measurements in Table 2. The seasonal dynamics of certain model parameters are presented and compared to actual results in Figure 1.

Table 2. Predicted and observed variables.

	Predicted	Observed	Units	Ref.	Note
Lake Superior					
Max.	0.05		mgC/l		
Phyto.	1.0	0.4-1.0	μgChla/l	17	obs. range
		≤1.0	μgChla/l	16	obs. max.
Max. Zoo.	0.01	0.018	mgC/l	21	from #/m^3
Max.	110	183	mgC/m^2/day	20	obs. max.
Prod.		76-507	mgC/m^2/day	20	obs. range
NO$_3$+NH$_3$	.26-.29	.22-.28	mgN/l	17	obs. range
Avail. P	0.1-1.0	0.5	μgP/l	17	obs. const.
Lake Huron					
Max.	.12	.03-.18	mgC/l	16	from wet wt.
Phyto.	2.4	1.2-2.4	μgChla/l	17	obs. range
Zoo. Range	.002-.012	.006-.058	mgC/l	24	obs. range
Max. Prod.	438	121-358	mgC/m^2/day	23	from hr^{-1}
NO$_3$+NH$_3$	.21-.26	.18-.26	mgN/l	17	obs. range
Avail. P	.15-3.0	.5	μgP/l	19	obs. mean
		2.0	μgP/l	19	obs. max.
Sed.	7.8	5.6	gC/m^2/year	22	north
Rate		15.1	gC/m^2/year	22	south
Lake Michigan					
Phyto. Peaks	.15, .06	0.2, .04	mgC/l	27	Gr. Trav. Bay
Max.	3.0	0.6-3.7	μgChla/l	16,26	obs. range
Max.	.012	.037	mgC/l	28	from ml/m^3
Zoo.		.2	mgC/l	28	nearshore
Max. Prod.	411	67-1030	mgC/m^2/day	16,26	obs. range
NH$_3$	.01-.028	.006-.024	mgN/l	27	Gr. Trav. Bay
NO$_3$	.22-.30	.1-.21	mgN/l	27	Gr. Trav. Bay
Avail. P	0.3-4.0	10.-3.5	μgP/l	26	
Sed. Rate	8.3	11.12	gC/m^2/year	29	assume 4% C (see ref. 22)
Lake Erie - eastern basin					
Max.	.28	0.1-0.4	mgC/l	16	from wet wt.
Phyto.	5.6	1.4-5.4	μgChla/l	30	obs. range
Max. Zoo.	.02	.06-.27	mgC/l	24	from dry wt.
Max. Prod.	775	140-1440	mgC/m^2/day	16	obs. range
NO$_3$+NH$_3$	.09-.19	.02-.18	mgN/l	17	obs. range
Avail. P	0.6-8.0	1.0-7.0	μgP/l	17	obs. range
Sed. Rate	11.6	160	gC/m^2/year	22	see text
Lake Erie - central basin					
Max.	.31	.06-.60	mgC/l	16	from wet wt.
Phyto.	6.2	2.-10.	μgChla/l	17	obs. range
Max. Zoo.	.03	.06-.27	mgC/l	24	from dry wt.
Max. Prod.	706	120-1590	mgC/m^2/day	32	obs. range
NO$_3$+NH$_3$	.05-.16	.02-.14	mgN/l	17	obs. range
Avail. P	0.7-9.0	1.-8.	μgP/l	17	obs. range
Lake Erie - western basin					
Max.	.83	.1-1.3	mgC/l	16	obs. range
Phyto.	16.6	4.9-25.9	μgChla/l	17	obs. range
Max. Zoo.	.07	.06-.27	mgC/l	24	from dry wt.
Max. Prod.	1026	110-1900	mgC/m^2/day	32	obs. range
NO$_3$+NH$_3$	0.3-.64	.08-.64	mgN/l	17	obs. range
Avail. P	0.5-25.	5.0-23.	μgP/l	17	obs. range

With a few exceptions the results of these simulations match the measurements quite well. The sedimentation rate for the eastern basin of Lake Erie (Table 2) is considerably underestimated. Burns[31] suggests that much of the eastern basin sediment originates in the western basin. The model prediction is based solely on material derived from the overlying water and does not consider horizontal transport; therefore, if Burns is correct our underestimate is to be expected. The prediction of sedimentation in the central basin is also considerably lower than that observed and the same mechanism may be operating. The most obvious failing of the model is in its inability to predict accurately the seasonal dynamics of the properties of the central and western basins of Lake Erie; this problem will be discussed in more detail below.

Lake Comparisons

In Table 1 the lakes are arranged in order of increasing trophic state according to predicted maximum phytoplankton concentration, sedimentation, and primary production. The ordering of the lakes based on our results agrees with trophic schemes reported in the literature[16,17].

The trend is also observed in predicted available phosphorus, especially the maximum values. Since phosphorus is generally accepted as the most common limiting nutrient in the Great Lakes, the increase in the maximum values is an accurate portrayal of the trend in trophic status. All of the lakes seem to have sufficient nitrogen available to the plankton; however, the trend in the minimum predicted value indicates that, as we look toward the more eutrophic lakes, the minimum inorganic nitrogen value decreases and the difference between the minimum and maximum values increases. The indication that the supply of nitrogen in the lower lakes is approaching levels critical to phytoplankton growth is also observed in the data compiled and reviewed by Dobson et al.[17] The effect of this nitrogen depletion is emphasized when one realizes that the average nitrogen half-saturation constant for phytoplankton growth is approximately 0.027 mgN/l[14,33].

Discussion

The results of the above simulations allow the lakes to be categorized in two groups: (1) those simulated quite well after minor recalibration of the Lake Ontario model and (2) those simulated less well and requiring further work. The upper lakes and possibly eastern Lake Erie fall into the first category, while the western and central basins of Lake Erie are in the second group. Examination of the lakes that fall in the two categories provides information on the generality and limitations of this specific model, as well as some implication of the requirements for models in general.

Upper Lakes

Although these lakes do have similarities (e.g., great size, climate, origin), they differ in trophic status and in aspects of ecological dynamics. Modeling a series of lakes of varying trophic status is analogous to modeling the eutrophication process in one lake. The ability of the model to predict accurately the levels of nutrients and biota in the upper Great Lakes lends credence to its potential generality; however, the fact that recalibration was necessary to obtain these predictions suggests that the model would not be able to predict accurately eutrophication within a lake without such recalibration. A model that was parameterized for phytoplankton adapted to the low nutrient levels in an oligotrophic lake would overpredict the outcome of enriching the lake. Upon increasing the nutrient levels, the algae as parameterized would grow excessively. In nature, algae outcompeted at low nutrient levels would succeed at higher levels because of other competitive advantages (e.g., size selective predation) and replace the oligotrophic forms. Multispecies models are required

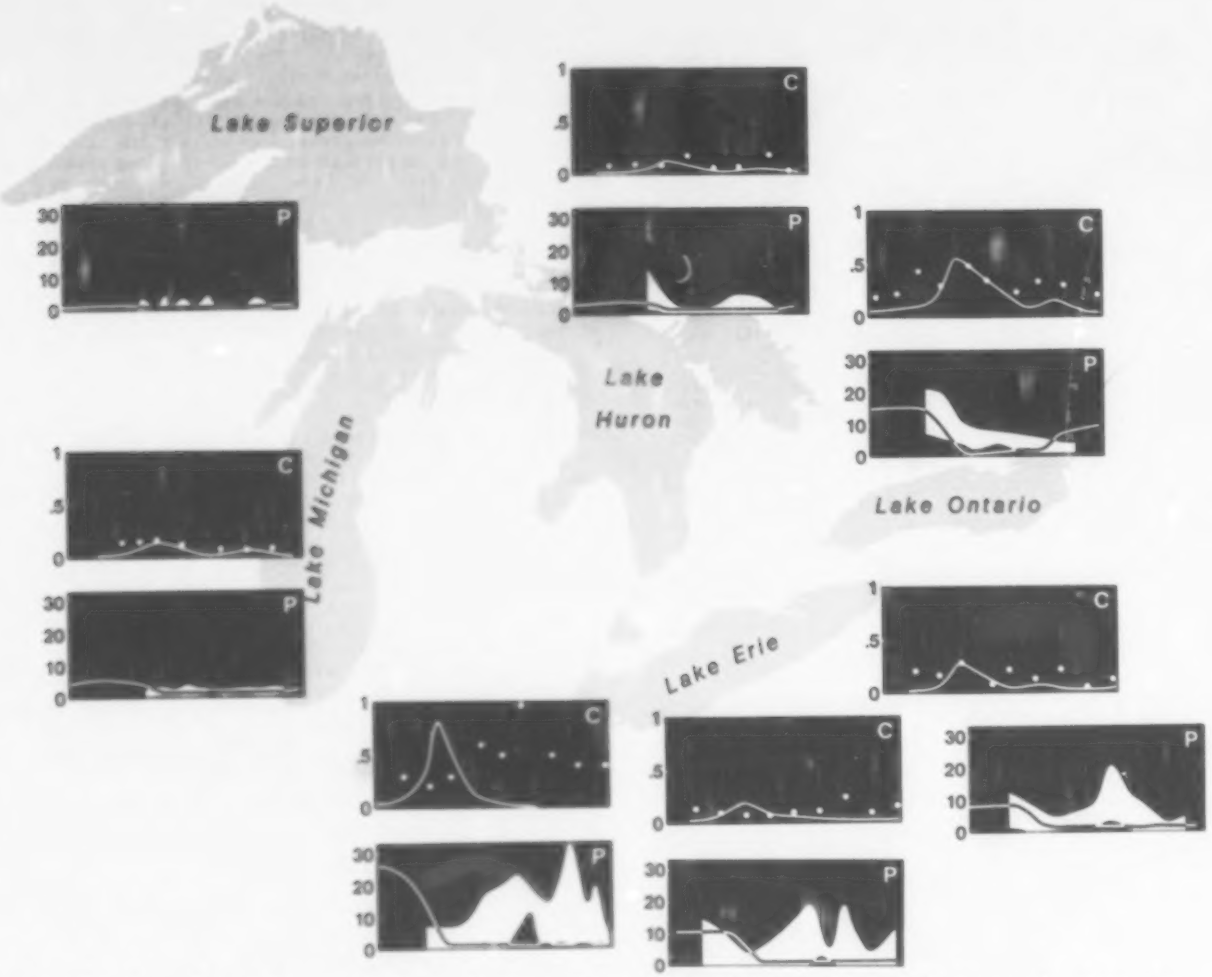

Figure 1. Comparisons of seasonal changes in observed and predicted values for phytoplankton carbon (C) and available phosphorus (P) for the Great Lakes with separate comparisons for the western, central, and eastern basin of Lake Erie. The predicted values for both C and P are represented by the lines. The observed values of C[16,25,30] (mgC/l) are represented by dots and the observed P values[35] (μgP/l) by the white areas which include the mean ± one standard deviation. The abscissa represents time from day 60 to 330.

to predict this sequence since single-species models cannot produce such succession.

To test this hypothesis, a simulation was run for Lake Superior with two of the four phytoplankton groups given a XKP value of 1 μgP/l and the other two a value of 9 μgP/l. This simulation resulted in almost exactly the same prediction for total phytoplankton as before; however, the algal groups with low nutrient requirements dominated and the ones requiring higher concentrations (XKP=9) were lost. This recalibrated model is not necessarily a general model, however, since it only accounts for one side of the competitive interactions at various trophic levels. We assume that in lakes with higher nutrient levels some counteracting competitive relationship favors the algal types that have higher nutrient requirements. The nature of this relation (or relations) is not clear at present, however, and so it cannot be added to the model. Even in this incomplete state of the model, however, our test indicates that multispecies models can mimic natural selection and, if the model is detailed enough to allow this succession to occur, can accurately predict the total phytoplankton biomass, as well as succession.

The need to change the second coefficient, XKG, implies the necessity for multispecies models of zooplankton. It also directs attention to the fact that very little is known about this coefficient and research should be directed towards its evaluation and determining what other processes are operating to affect succession during eutrophication.

The development of multispecies models may not be the only alternative available to simulate eutrophication. Another method could be to make the important coefficients functions of the environment. Allowing XKP, for example, to change as a function of phosphorus concentration is one way to simulate adaptations of the phytoplankton community. Although this method may be more easily implemented, we feel multispecies models will be more realistic.

Lake Erie

The Lake Erie simulations were generally less successful than those for the upper lakes. This limitation of the model suggests that ecological models will often fail when applied outside the physical realm for which they were developed.

The failure in the central basin was most attributable to not accounting for the special processes associated with anoxic hypolimnetic conditions. Under anaerobic conditions in Lake Erie, the regeneration of phosphorus from the sediment is approximately 11 times greater than under aerobic conditions[34]. As a result of ignoring this process, the seasonal dynamics of the biota of this basin were not simulated accurately; and the phytoplankton concentrations were grossly underestimated during late summer and early fall, when the sedimentary regeneration occurs.

The western basin is also greatly influenced by physical properties not considered in the model. Allochthonous loadings to the large, deep upper lakes probably do not affect the seasonal dynamics, whereas the episodic inputs to western Lake Erie, which has a short residence time, certainly affect the biota. Also, the shallow basin would be perturbed by any relatively high intensity winds, resulting in resuspension of sediment. This process and anoxic release of sedimentary phosphorus are not included in this version of the model, and we feel these omissions have resulted in the poor predictions for this basin.

Conclusion

We feel that this analysis points out that models built to describe the ecology of lakes can be general enough for use in a range of situations; however, they will have to include multispecies compartments in the food web in order to simulate natural succession. To accomplish this end, substantial efforts are needed to describe and document the processes critical to the ecological models at the "functional species" level.

This study also emphasizes the need to analyze critically a body of water before developing a new model. In many cases only the physical processes of a model (depth, stratification, sediment/water exchange) need to be altered to adapt a preexisting model.

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Simulation and Mathematical Modeling
# of Water Supply Systems - State-of-the-Art

Rolf A. Deininger
School of Public Health
The University of Michigan
Ann Arbor, Mich. 48109

SUMMARY

Mathematical Modeling and Simulation Techniques have been used extensively in many parts of the overall water supply system ranging from the actual abstraction of water from ground and surface water sources, to the primary collection and conveyance system, the water treatment plant and the final distribution system. The following areas have found attention:

Population projections and forecasts of demand
Design and Operation of Wellfields
Regional Water Supply Networks
Design and Operation of Treatment Plants
Design and Operation of the Distribution System

Population Projections and Forecasts of Demand

This very important aspect of water supply planning is covered elsewhere at this conference and will not be treated here.

Design and Operation of Well Fields

In the design and operation of well fields several aspects are of interest. The first one is the following: given an areally extensive aquifer, how many wells of what size should be placed where and how should they be pumped to obtain the required yield from the field at minimum total cost? The second level of the problem is: given an existing well field, how should it be operated for maximum yield, or given the required yield, how should it be operated for minimum cost of production.

The first of the above problems is the more difficult one, since it involves the process of selecting the number, type, and location of wells. An approach in this direction has been shown in a paper by Aguado[42] involving an optimal plan of dewatering a construction site. The flow of water in the aquifer is described by finite-difference approximations of the governing differential equations. The problem is then formulated as a linear programming problem which determines the necessary amount of pumpage from the wells which arranged on a grid line. Both steady state and transient conditions were investigated.

The second type of problem, namely the operation of a well field, has been investigated by Deininger[46] and also Aguado _et al_.[43] Linear programming techniques were used to determine the optimal pumping from a given set of wells, subject to pump limitations, boundary drawdown limits, and aquifer characteristics.

Regional Water Supply Networks

The major problem addressed in these studies is the development of sources of water supply and the delivery of the water to the points of consumption. Typical of these studies is for example the one by Carey[7] who studied the water transfer in the New York Metropolitan area, the one by Deininger[46] who described algorithms for the optimization of regional water supply networks. The basic problem can be stated as follows: Given a number of surface or ground water sources, which of these sources should be developed at what time and to what extent and how should that water be treated, stored and transported such that the needed quantity and quality of water will be available at the demand points and the total costs are reduced to a minimum.

The major design variables are the number, size and location of surface reservoirs, including their elevations; the size, number and location of wells in a well field; the routing, number and sizes of the transmissions mains including the pumping stations; the treatment of the water to make it potable; and finally the rules of operation of the system.

The formulation of the above problems leads to typical network problems and a variety of algorithms, mostly linear and nonlinear programming have been used to analyze the problem.

Two further studies which are worth mentioning are those by Young and Pisano[41] and a study by Weddle[40]. The study of Young focuses on the James River and estuary and the water supply to the cities of Richmond and Hampton Roads. A variety of sources of water is considered, such as surface water, ground water, brackish water, sea water, and renovated waste water. The major decision variables are the surface water reservoir, the location and number of wells for tapping the ground water, the location of a possible electro-dialysis plant and a desalination plant, the location and type of a waste water renovation plant, and the necessary pipe lines for transferring the waters. The entire quantity and quality problem was formulated as a nonlinear programming problem, and was solved under different assumptions for costs and technology to identify the most promising solutions. The study by Weddle focuses on an unspecified coastal situation, and again the elements of supply considered are conventional surface water, seawater desalination and wastewater renovation. The demands are municipal, industrial and agricultural. The resulting mathematical programming model was a mixed integer programming model, and several good solutions were generated.

Design and Operation of Treatment Plants

At the treatment plant level the questions arise as to what type of treatment is necessary, what combination of units is required, and how a minimum cost treatment plant can be designed. There are very few attempts in the literature to formulate this as an optimization problem, and the few existing studies appear to be more on an academic level. On the other hand the capacity expansion of a plant has found greater attention, as shown by other papers here at this conference.

Design and Operation of the Distribution System

This area of a water supply system has attracted by far the most studies. While the earlier work has been mostly in trying to balance the flow in the network, the newer ones attempt to design a least cost network which satisfies the demand and pressure requirements. Several good methods and algorithms exist, although from a strictly mathematical point of view we still lack a method for designing a least cost network. The basic questions of network connectivity and reliability should also warrant more attention.

For all the above-mentioned areas of modeling the dynamic and time aspects must be taken into consideration, which means a study of the capacity necessary at a given time, looking over a finite planning period. This gives rise to the typical capacity expansion problems and the sequencing of the construction of individual parts of the system.

Towards a Drinking Water Quality Index

The Public Health Service Drinking Water Standards were first adopted about 60 years ago to protect the health of the traveling public. In 1946, 1956, 1962, and again in 1975 amendments and revisions were made to reflect the changing environment and new knowledge about what substances to expect in water and what concentrations are thought to be allowable. And thus the "Safe Drinking Water Act" (PL 93-523) calls for new standards on the maximum allowable concentrations of substances in drinking water.

Any water supplies not meeting the new standards will be subject to the provisions for correcting the situation, but the interest should be on those water supplies which meet the standards. Among these, there must be some which are better than others. The basic question is how to rank them, and if such a ranking would be undertaken, whether or not one would see a difference in the quality of the supplies.

In an attempt to see if a ranking is possible a printout of the data of the Interstate Carrier program was obtained which lists values for 24 parameters of water quality. In an attempt to stratify one city from each of the 52 states was selected only guided by the principle that as many parameters as possible should be available.

Each of the parameters has a single numerical standard. Thus, for example, the concentrations for lead and mercury are .05 and .002 mg/l, respectively. It can be argued that none of these substances are needed by the human body, and that the most desirable value would be zero. In other cases, for example, sulfates, it was felt that while the standard was 250 mg/l, a desirable value would be about 35 mg/l. In other words, for each parameter there exists a standard and the most desirable value, the latter being usually zero or lower in concentration than the standard.

An average index can then be calculated which measures the degree by which a particular water is close to the desirable concentration levels. Such an index formulation was applied to the data, and a ranking of the supplies was possible and showed the wide differences in quality.

Conclusions

Mathematical Modeling and Simulation techniques have been used in practically every aspect of a water supply system. The number of studies and applications in the design of well fields appears to be rather limited, and some further concentrated effort appears to be in order. In the area of regional water supply systems several models exist, and the practice of carefully evaluating alternatives seems to be standard practice. Direct optimization of the design of treatment plants and the operation of them is rather limited and seems to be constrained to academic exercises.

The design of a distribution system has attracted many studies, and at the present time good algorithms exist, although from a strict mathematical point of view none of them guarantee the global optimum. Basically, the use of mathematical models and simulation techniques such as linear programming, dynamic programming, etc., aids in the analysis of water supply systems in four major ways:

1. It allows the analysis of more alternatives at every level of decision-making;
2. It allows a better testing of the assumptions and estimation of the influence of economic, political and environmental uncertainties;
3. It provides a mechanism whereby all assumptions and judgements are made explicit and are clearly laid out, and
4. It serves as a communication tool for alll the professionals involved in water supply systems planning.

An extensive literature exists, as shown on the pages following. It is up to the profession to put it into practice.

Note: Due to space limitations only a brief summary of the paper is presented here. A complete paper is available from the author.

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CAPACITY EXPANSION FOR MUNICIPAL WATER AND WASTEWATER SERVICES:

INCORPORATION OF UNCERTAINTY

Robert G. Curran
President, Curran Associates, Inc.
Northampton, Massachusetts

David H. Marks
Resource Analysis, Inc.
Cambridge, Massachusetts

Donald S. Grossman
Resource Analysis, Inc.
Cambridge, Massachusetts

Summary

Methods for management of local water and wastewater investments are outlined. The strategy is to choose the least cost supply alternative that services a forecast but uncertain equilibrium demand. Careful attention is paid to the overall usability of the method by local planners.

The research defines water and wastewater service demands, and identifies some controls available to local decision makers for modification of these demands. The level of future requirements for planning is uncertain; the form and magnitude of the uncertainty is explicitly included. Supply alternatives and forecast costs of supply are also presented. Forecasts are developed for local relevance and to best utilize available information.

A detailed analysis of time phasing and scale of capacity expansion requires forecasts of the impact of supply shortage. Short term alternatives in shortage can either act to limit demand or to increase supply. Recommended cost assessment for these strategies is empirical. The criterion for expansion planning is to choose the alternative which minimizes total costs, where costs include construction, operating, and shortage penalty fees. The recommended expansions explicitly incorporate forecast uncertainty in the evaluation of alternative investment patterns.

Problem Description

Municipal water and wastewater investments represent a large and important segment of the capital expenditures made by local governments. The traditional response of designers to the problem of sizing increments of capacity has been to build for arbitrarily long planning periods, that is, to overbuild in order to assure safe and adequate supplies. This is due, at least in part, to the relatively naive approach presented by traditional engineering textbooks and required by Federal funding guidelines. A growing body of evidence indicates that overbuilding is not the best response to the uncertainties inherent in future demands for service. Two basic reasons may be cited. First, oversized system elements are not economically efficient. Second, water resource related investments may have impacts upon whether or not land is used, and for what purposes.

Public water supply and wastewater disposal is undertaken for a variety of reasons. Commonly accepted considerations for municipal provision of water supply and wastewater disposal include public health, public safety, resource regulation, land use regulation, and economic efficiency. Given the basic premise of providing water related public services, the local decision maker still has a range of options that define the extent and quality of service. The character of service depends also upon the sorts of demands, and the consequences of not meeting those demands.

The immediate decisions available include size and location of water distribution or sewer collection mains, the size and location of treatment or supply facilities, pricing or metering policies, and the types of users and uses allowed. Some of these, especially those related to sizing capital facilities, are generally made in the long term in order to take advantages of the economies of larger developments. Others, such as changes in pricing or allowable uses, are easily changed on a short term basis.

Demand has important effects upon the quality of the services offered. In order to size the supply, the factors which influence demand for service, and the magnitude of the influence, must be ascertained. It is relatively recent that an outstanding of the elasticity of the demand for water has been established. Also, the consequences of not meeting demand must be thought of in realistic and unemotional terms. Shortage of supply need not result in unsanitary conditions or shortage of water for drinking. Rather than restricting the availability to always meeting demand, planning should exhibit some sensitivity to the costs of not meeting demands.

The traditional engineering approach may be briefly characterized as supply oriented. The steps are to project demand, and then to find the least cost supply to satisfy demand. There are several shortcomings with this approach. First, methods for demand projection including curve fitting or graphical analysis are naive in that they only preserve past trends in the data. Second, the method limits the range of study to structural rather than nonstructural alternatives (e.g pricing). Third, demand is assumed as a given, no matter how much it costs to satisfy that demand: that is, planned inadequacies or shortages are ruled out. Fourth, arbitrary design horizons are often set, which ignore the tradeoff between economies of scale and the cost of capital.

More generally, a large number of inputs necessary for decision making are uncertain. These include future demands, cost of addition to supply, costs of shortage, and interest rates. In order to effectively plan in an environment of uncertainty, the analyst must understand the sensitivity of system objectives to variations in policy. If the output does not show much response to input assumptions or policies, then despite uncertainties or policy changes, then the uncertainties are of little concern. If the outputs are sensitive, then the analyst may collect more data, remodel the planning process, or try to explicitly model the uncertainties.

Model Framework

The framework proposed for planning in this paper is basically a least cost supply model. The simplest case to plan for is the expansion decisions for a single facility, for example, a single link in a pipe network, or a single treatment plant. A key assumption is that there is an identifiable service area. The steps proposed for planning in such a case are to:

(a) Forecast demand

(b) Estimate costs of expansion of supply

(c) Estimate costs of shortages

(d) Decide on the increment of plant capacity, and the timing of these increments, based upon forecast demands, and the costs of meeting or failing to meet forecast demand.

Rather than ignore the uncertainties that are known to exist, and are universally agreed upon, an effort is made to focus upon the forms and degree of uncertainties. The philosophy is that this enables the analyst to use more of the information available for planning.

Unfortunately, it is difficult to check the validity of this method, except through in depth studies of field experience with the planning tool. These have not been possible within the limited time horizon of this research. Rather, the proposed approach is to see how the model results compare with models using differing input assumptions. For example, one test would be to compare total system costs and investment strategies assuming certainty, and then assuming uncertainty in demand, all other things being equal. The output from tests such as this should better enable the analyst to choose a method which matches his understanding of the problems in planning water and wastewater investments.

Demand Analysis and Forecasting

The traditional methods of demand forecasting by naive trend extrapolation are reviewed in several references (4, 32, 36, 37), but McJunkin's article (32) is the classic study for civil engineers. More sophisticated models require some understanding of the causality of demand processes. The view of demand for service taken in this research is that of a heirarchical process of development, inhabitation, and consumption.

Models for understanding the development process are numerous, and readily found in the transportation or urban planning literature. It is anticipated that developers look at sites from the same viewpoint as households or businesses that seek to locate. The developers seek sites consistent with the preferences of the groups to whom they are trying to market. A theoretical basis for understanding residential location is well developed. Alonso (3) postulated that budget constrained households choose a site that maximizes their utility, where utility is a fraction of amount of land, commuting costs, and composite measure of all household goods. A number of models have been developed for forecasting on this basis (17,23,42). The theory of location of the firm is less well developed.

Although this describes the relative attractiveness of locations within a region, it in no way provides a rationale for the driving force behind growth in population, or differences in growth between regions. Therefore, the usual approach is to forecast population and employment on a regional level, and to allocate the forecast within the region.

As early as 1963, research (39) showed that sewer service was significant in inducing conversion of vacant to developed land. Later, it was shown (24) that an index of utility availability explained interregional differences in growth. More recent studies (13, 14, 44, 45) have attempted to quantitatively model the impact of wastewater infrastructure investments. The state-of-the-art ability to model the magnitude of development changes is limited. Key drawbacks of the models include strong data dependence, and the unavailability of accurate projections for the parameters that force or drive the output. Rather, the importance for the analyst or planner is careful recognition of water or wastewater policy relationships to development.

Given an equilibrium developed stock of residences, stores, offices, and industrial sites, consumption depends directly upon the degree to which the stock is utilized. Normal vacancy rates for residences are approximately 3% (21); in some urban care areas the vacancy rate can be dramatically above 10%. The important observation is that even if developed stock can be accurately inventorized, this need not be a good indicator for assessing consumption.

Conditioned upon development, and then upon inhabitation of an area, the total water and wastewater supply required is determined by both level of service offered and by individual consumer demand characteristics. The ensuing discussion emphasizes that water and sewer services can and should be treated as economic goods. Level of service changes can cause shifts in demand, and, similarly, the preferences of consumers can change over time.

Different elements of the system must be designed to satisfy different components of demand. Demand for water exhibits daily, weekly, and annual cycle variations. Annual cycles are important for planning basic source; demands on the maximum day are important for planning transmission, facilities, treatment facilities, distribution pumping stations, and major feeder mains; peak hour demands or maximum fire flow are important for planning local distribution mains, connections, and local storage. Wastewater demands typically exhibit a close relationship to observed water demands. A number of crude rule-of-thumb multipliers are available for relating demand components.

Four district classes of user generally cited in water and wastewater planning are residential, commercial, industrial, and public unaccounted uses. Research on residential water usage has been extensive (15, 16, 19, 20, 25, 42, 44, 46). The basis for most of the studies cited is, at least indirectly, a project to study residential water use conducted at Johns Hopkins University. A summarization of the project results is presented in a paper by Howe and Linaweaver (20). The Howe and Linaweaver study concludes that residential users respond to price as a quality of service indicator. The importance of this sort of research is in quantification of the effects that changes in level of service can have on demand. It provides a basis for analysis that is readily applicable and easily reproduced, and helps guide in the formulation of level of service policy charges.

Unfortunately, due to a lack of transferrable models and data, the most convenient way to forecast demand for service is to project population, and then to apply population to use multipliers. Two points must be emphasized. First, the focus need not be on the development of better point estimates for future population levels, but instead on a quantification of the uncertainty in population forecasts. Second, the analyst should, as much as possible, utilize locally-based consumption data in calibrating use multipliers.

The traditional engineering texts have paid painfully little attention to the subject of demand forecasting. A study by James, Matalas, and Bower (22) shows, for one particular system, the economic development projection to be the most important variable in water resources planning, yet many current texts still propose graphical extrapolations or simple regressions as the basis for demand forecasts. A method for dealing with this dilemma is to make several projections, and perform an ad hoc sensitivity analysis. If, in fact, investment planning decisions are shown to be sensitive to economic development projections, as expected, then the analyst must in some way combine the information from several projections in order to formulate an investment strategy. Rather than choose between projections in some arbitrary fashion, the analyst might consider trying to model the likelihood of the projections.

Several models of this type for modeling population growth as a stochastic process are available and easily applied (5, 28, 33, 34, 35). Limited evidence shows that the stochastic model performs better in capturing the variance of the underlying population growth (34). Often, this is severely underestimated by regional planners. A common formulation is to model birth, death, and migration rates as stochastic processes. First, a form for the process is chosen. Second, process parameters are estimated using historical data. Third, the observed parameters and chosen form are used to simulate future population growth. Fourth, a distribution form is chosen, and statistics gathered on the uncertainty in future population levels. This modeling approach uses data available more frequently than census data, so process parameters may be estimated with greater confidence. Also, the method has causal structure which allows for improvements beyond those possible with aggregate population models. One important area for future research is extension of the basic model structure to use subjective or regional information in a Bayesian fashion. Another is the refinement of models for use in regions with dependent subareas. The use of stochastic population models seems to be a promising area for additional research.

Population is only a surrogate for the desired metric of demand for water or wastewater services. The proposed method is to convert stochastic population forecasts to demand forecasts through the use of consumption multipliers. Standard multipliers are available in a number of sources (19). These do not account for consumption habits, pricing effects, climate, and other factors which can cause variations in water or wastewater production. Therefore, the analyst should endeavor to gather local data to estimate consumption multipliers. Care should be taken to include the component of demand due to infiltration, inflow, or leakage (4, 19). A preferred method, to model the variation in observed use, is not possible due to the lack of data and lack of theoretical framework.

Supply Analysis

The choice of supply alternative depends upon the type of demands being planned for, and upon the site characteristics of climate, topology, geology, and existing or planned development. The choice of supply will also depend upon the relative costs and upon the availability of supply alternatives to satisfy demand. A key assumption taken in this analysis is that the cost function for the current project is independent of the number and sizing of projects preceding the current decision. In other words, the cost function for system expansion appears identical at all points in time.

Within the analysis of water or wastewater facilities, the planner can choose the depth of analysis. The simplest approach for facility analysis is to determine a functional form for the costs of expansion, and then to utilize standard parameters to determine the exact scaling of the function. A more sophisticated approach is to use observed or synthetically generated points to calibrate the cost function parameters. Both of these methods will be reviewed in this section. It is important to note that due to the strong dependence on site characteristics, local calibration of parameters is the preferred alternative.

In general, over a wide range of sizes, water and wastewater system elements exhibit economies of scale: it is possible, however, to get out of the range of economies. The most commonly used representation for a cost relationship of this sort is

$$C = kQ^m \qquad (1)$$

where C is the total cost (usually in dollars, k is the scale parameter, Q is the total capacity, and m is a scale parameter. This relationship exhibits economies of scale for values of m between zero and one. Observe that the function is continuous, suggesting that the equipment is available in any sizing. Although in practice, this is not possible due to standardization of components or to site irregularities, it seems to be a reasonable assumption that helps improve analytic tractability.

The two parameters have been estimated for a number of system elements. These estimates have been taken, in general, from two sources of information. One way to estimate the parameters is to use a broad base of observed costs and installed capacities, and use regression or some other curve fitting technique. A second way to develop a basis for fitting the cost function is to synthetically cost a number of alternative installation sizes, and to fit a function to the synthetic data. The latter method is useful in trying to develop cost functions with local significance. Examples of parameters in the literature are numerous (1, 2, 4, 5, 7, 8, 9, 10, 18, 27, 36, 40). The variation in reported parameters reflects a number of differences in data or underlying assumptions. The comparisons may be misleading due to site specific differences. Also, units may be incommensurate due to misadjustment for exchange level or technology.

Site specificity is of primary importance. Clearly, the costs of capacity depend heavily upon the relative suitability of sites for development. The above model assumes the only difference between projects to be size. Variation in cost could also be due to hydrology, topology, geology, existing development, planning development, durability of installation, site aquisition, legal, construction materials, site preparation, and so forth. Any number of these might be included as explanatory variables if the data were available and if they could be forecast for future planning: neither is the case. A suggested approach, therefore, is to try and qualitatively control for sources of variation other than size. This would require definition of categories exhibiting significantly different cost parameters, and estimation of those parameters for use in a look-up table. Neither the data nor the theoretical basis exist to accomplish this. In the interim, generalized scale factors are the only alternative to site specific cost assessment.

Differences in costing assumptions or accounting stance may also explain variations in scale factors. The parameters are based solely on primary construction costs, and no secondary environmental or socioeconomic impacts are included. Other accounting issues include transformations between currencies and intertemporal comparisons. These require choice of a suitable exchange rate and discount rate for transformation to a common datum. Another accounting issue is the problem of inflation of water and sewer prices differing from the general rate of inflation. In the case of water and sewer plant, the ENR index has been increasing at a rate of 5.5 percent per year, while the consumer price index has increased at a rate of 2.8 percent per year. A correction must be made to reduce the opportunity costs of capital by the rate of relative price increase.

Thus far, little attention has been paid to the definition of the quality supplied. Assuming a design configuration (and operating policy, if applicable), the level of supply is variable due to climatic variations or reliability problems, and there is typically some probability that the source installation chosen will not satisfy demand. The usual method for treating this is to consider component reliability for a certain confidence level. If possible, sensitivity analysis should be employed to test the validity of the reliability level chosen.

Finally, a simple analytic form was chosen for the cost function. The capacity expansion model, in its most general form, does not require an analytic cost function. The models developed in this research may be readily generalized for use with any monotonic cost function. However, this has not been fully implemented in this version.

Costs of Shortage

Estimation of the costs of shortage is a new and an important area for research (40). The key concept is that the costs of shortage are not infinite. Shortage may merely imply inconvenience or it may mean a much more serious condition. Adjustments can sometimes be made by consumers in order to lessen the impact of shortage. This section discusses the types of adjustments possible, and considerations for estimation of the costs of these adjustments.

Most engineers and utility managers accept the premise that systems should be designed to accommodate demand at all times. Shortfalls are not acceptable, and should, therefore, be avoided with accurate forecasting, planning, and (over) design of facilities. Implicit in this approach is the assumption of an infinite cost of shortfalls in supply capacity or in delivery capacity. One suspects the true costs to relate to the adjustments that are possible.

Adjustments in the case of shortage may be categorized as either acting to increase supply or to reduce demand. For water, measures that increase supply include emergency storage and interconnections with other systems. Measures that reduce demand include changes in pricing, changes in the pricing mechanism (e.g. the installation of meters), restrictions on uses (e.g. lawn watering or car washing prohibitions), and restrictions requiring reuse (e.g. recirculating air conditioning equipment). Note that adjustments that reduce water demand affect both distribution and source shortage. For sewer, measurements that increase supply include inline storage and flow regulating devices. Measures that reduce demand are expected to be similar to those used for water supply.

The major study of supply shortage is that of Russell, Avery, and Kates (40), who have documented productivity losses for several Massachusetts communities during the Northeast drought from 1961-1966. Their general methodology defined water-shortage losses as "gross annual benefits lost by disappointed users less costs avoided by the supplier." The authors assumed full employment and assigned costs to the resources diverted to meet a drought crisis. The calculation of actual losses was corrected in several ways to reflect different interest rates and accounting stances. In cases where firms deprived of normal quantities of water undertook investments in water conserving technology, it was counted as a benefit. In a number of cases, the net result from a national point of view of the effect of drought on commerce and industry was that the investment in water saving technology produced a benefit rather than a cost.

Observed losses were related to the percent shortage, which was in turn related to the measure of system inadequacy. Two difficulties arose. First, system managers' anticipation of shortage caused costs to be incurred without shortage having actually occurred. Second, existing safety factors were not known. None the less, an exponential cost function was estimated.

There is strong reason to believe that the loss relationships will differ for different geographical sections of the country and for areas with differering levels of usage in industrial, commercial, domestic, and municipal sectors. For example, cost of drought could be significantly higher in more arid areas.

Overall, the work of Russell, Avery, and Kates is an excellent effort in quantifying an elusive relationship. More work needs to be done to verify the results, and their transferability. A significant effort must be made to obtain similar results for the costs of wastewater service shortfalls. Analysis of capacity expansion investments should help quantify the sensitivity of total system costs to the costs of shortage.

Capacity Expansion Decision Making

Given demand forecasts, costs of expansion, and costs of shortage, the final planning step is the choice of timing and sizing of increments for supply expansion. This problem is closely related to the inventory control problem, and a number of models have been proposed in the literature. This section discusses the available models, including several new applications to water and wastewater planning. A number of models are presented to allow the user a considerable degree of flexibility in the depth of analysis undertaken. This also allows for the added ability to incorporate uncertainty in demand, or not.

There have been two classes of research in this problem. One is the choice of a finite set of projects with known costs and supply potential, and simple sequencing of these projects to meet forecast demand at least cost (11, 30, 31). This approach requires the solution of a combinatorial problem, and the feasibility of solution depends heavily upon the number of projects under consideration. The advantage of this method is that it takes account of the exclusivity of projects. The disadvantage, which is overriding, is that the choice of projects, and their sizes, is made independently of rather than simultaneously to the sequencing problem. This hierarchical decision process can be suboptimal. The second approach (5, 6, 7, 12, 18, 26, 28, 29, 38, 40, 41) is to choose the timing and sizing of capacity increments to satisfy demand at least cost, where demand may be uncertain, and where the costs may be due to construction, operation, maintenance, and to shortage.

Eight models are proposed for a planning package. These include varying assumptions about linearity or nonlinearity and certainty or uncertainty in demand. They also include varying assumptions about allowability of shortages. Table 1 shows a categorization of the models.

	Certainty	Uncertainty
Linear	Shortfalls no Shortfalls	Shortfalls no Shortfalls
Non-Linear	Shortfalls no Shortfalls	Shortfalls no Shortfalls

Table 1: Model Typology

The reason for considering this broad a set is that the simpler models, for example certain linear demand with no shortfalls, have closed form or very efficient solution procedures. The more complex models, for example nonlinear uncertain demands with shortfalls, require elaborate solution procedures such as stochastic dynamic programming. The analyst interested in extensive sensitivity analyses could, therefore, sacrifice the greater realism of the more complex models for the efficient soluability of the simpler model.

All four cases of model assuming linear demand have been studied extensively by Manne (28, 29), and several have been applied in planning water or wastewater investments (5, 6, 26, 38). The assumptions that go into these models are all similar. The assumptions include infinite economic lifetimes for projects, an infinite planning horizon, and no budget constraints. For the cases of uncertain future demands, a Bachelier-Wiener diffusion process in continuous time is used as the model. The form of expansion costs is $C = kQ^m$. Operating and maintenance costs cannot be included in these models. Costs of shortfalls are linear in the magnitude of shortage. Although these assumptions result in a highly simplified model of the capacity expansion planning process, the advantage is that the models have closed form solutions or require simple one or two dimensional searches.

Using these models, the sizing of capacity increments has been found to be sensitive to discount rates, economy of scale parameters, demand, and demand uncertainties. The indication in research by Manne is that lower discount rates, or higher economy of scale parameters, leads the analyst to recommend larger investments in capacity installments. The exact nature of the relationship between time that the investment should supply, economy of scale, and the discount rate is available in several published sources, including Manne. When the penalty cost is assumed to be infinite, that is, no shortages are allowed, and in the case of demand uncertainty, Manne indicates that one should overbuild, as compared to the case of certainty. When the shortage penalty cost is less than infinite, no definite results have been drawn.

The four cases of model assuming nonlinear growth in demand have not been dealt with as extensively. The only related study in the water and wastewater planning literature is that of Russell, Avery, and Kates (40) which reviewed costs of shortage for the mid-1960's New England drought. The model used to optimize investment strategy for deterministic demands was a nonlinear programming algorithm. The assumptions included deterministic demands, infinite economic lifetimes for projects, expansion costs for the form $C = kQ^m$, shortage costs quadratic (or greater) in the magnitude of shortage, no budget constraints, and no operating or maintenance costs.

Two uses were made of the model. It was applied, ex poste, to judge the quality of water supply investments for several New England towns. This is somewhat unfair because it uses information on population not available at the time the actual decisions were made. The model was also applied to develop prototype rule of thumb guidelines for investment planning by local decision makers. Results were represented in terms of a dimensionless level of inadequacy, defined as the ratio of 'current' use to safe yield. Based upon input assumptions about the discount rate, shortage costs, and economies of scale, the tabulated results indicate the level of inadequacy at which to build, and also the length of planning period for which to build. Higher discount rate, higher economies of scale, or higher shortage costs all lead to the recommendation to build for shorter planning periods, and vice versa. The research does not, however, provide insight into the value of modeling nonlinear demand growth as compared to using a linear approximation to the growth in demand. It does show that if demands are uncertain then total system cost is sensitive to the costs of shortage.

The solution procedure was a nonlinear programming algorithm based on the method of Zoutendijk. A number of combinations of loss function parameter, scale parameters, discount rate, population growth rate, and per capita consumption growth rate were studied. Total costs were fairly insensitive to the loss function parameter, but highly sensitive to the discount rate. Not only did costs change with differing discount rates, but capacity increment sizes also changed. The total costs were sensitive to economy of scale parameter but the sizing of increments was less sensitive. Overall, the model provides a basis for analyzing nonlinear growth in demand with shortage.

It can be shown that capacity expansion decisions for an arbitrary monotonic demand path can be modeled as a dynamic programming problem. For the cases with shortage, this simply requires a suboptimization step. The dynamic programming problem formulation can be readily solved using any of a number of efficient shortest path algorithms. To expand the nonlinear demand model to include cases of uncertainty in demand, a stochastic dynamic programming formulation can be established. This is related to previously studied stochastic inventory control models. The distribution on demands is generally discretized. Models of this type have yet to be applied to planning water or wastewater investments.

For the nonlinear demand models, the additional complexity of a budget constraint may be introduced. Similarly, restrictions on available plant sizes and maximum allowable shortages may be included. The form of cost and shortage cost functions may be varied, and operating and maintenance costs added. All of these are relatively straightforward but as yet untried extensions.

Conclusions

There is no general availability of a set of models for forecasting demand, estimating expansion costs, estimating shortage costs, and planning capacity expansion for water and wastewater investments. Such models in a usable package would provide municipal decision makers with the flexibility to model in a simple sketch planning fashion, or the ability to model more complex assumptions about the underlying system. Rather than develop a single plan for capacity expansion, a range of plans might be developed. Sensitivity to input assumptions, or the underlying distributions of input variables would aid in incorporation of the large uncertainties inherent in planning social systems. Ultimately, these might be abstracted to provide simple rules of thumb for planning.

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ADAPTIVE SHORT-TERM WATER DEMAND FORECASTING

David H. Budenaers
Systems Control, Inc.
Palo Alto, California

Summary

A dual set of short-term water demand models is described. These models have the feature of adaptability to changing data. That is to say, given changes in the data sequence, the models' parameters will self-adjust to provide a better model. The models also have the property of being real-time computer-implementable.

The two models are a stochastic (or time-series) model and weather component of demand model. The stochastic model is an extension of the Box-Jenkens type of modeling for time series. The weather model uses the method of principal components to identify the effective weather variables.

The results of the application of these models to data from the San Jose, California, Water Works are presented.

Background

Demand forecasting is of central importance for the development and implementation of a methodology for design and operation of water distribution systems because it forms the basis for developing operational policies for [1,2]:

- Storage management
- Scheduling of sources of water production.

The methodologies selected for implementation in the demand forecasting algorithm are of two types:

- Stochastic models
- Weather model methods.

Stochastic methods make use of the historical empirical demand time series to predict or extrapolate the future. Stochastic methods attempt to explain the demand time series by using the series' internal correlation structure without use of any external or explanatory variables. In order to implement a stochastic model, a detailed statistical analysis of the time series' correlation structure must be performed.

For example, it must be determined if, as a rule, today's water demand is highly correlated with yesterday's demand.

On the other hand, weather models try to explain the demand time series by use of external variables. Intuitively, the most predominant external variables to affect water demand are weather variables. Thus, in weather models, a detailed study of the relationship between weather variables and water demand must be implemented.

Once the relationship between weather variables and water demand has been identified, then it becomes possible to forecast water demand based upon weather predictions.

The Stochastic Model

An examination of typical demand data for water demand (Fig. 1) suggests that a high-gain stochastic model could model the demand time series. The term "high gain" means that the internal correlation, described in the previous section, is highly adaptive to new data. In light of this fact and the fact that stochastic modeling has proven to be successful in other similar applications, the following model is proposed [3] :

$$D(t) = B(t) + X(t), \qquad t = 0, 1, 2, \ldots \tag{1}$$

$$X(t) = a\, X(t-1) + u(t), \qquad t = 1, 2, 3, \ldots \tag{2}$$

where

$D(t)$ is the demand at time t

$B(t)$ is the base effect at time t

$X(t)$ is the autoregressive term given by (2) (autoregressive lag one)

$u(t)$ is a sequence of independent random variables where $E[u(t)] = 0$, and $\mathrm{Var}[u(t)] = \sigma^2$.

Both a and σ^2 are unknown parameters. In addition, B(t) is an unknown quantity.

Observe that

$$E[D(t)] = B(t) \tag{3}$$

$$\mathrm{Var}[D(t)] = \frac{\sigma^2}{1-a^2} \tag{4}$$

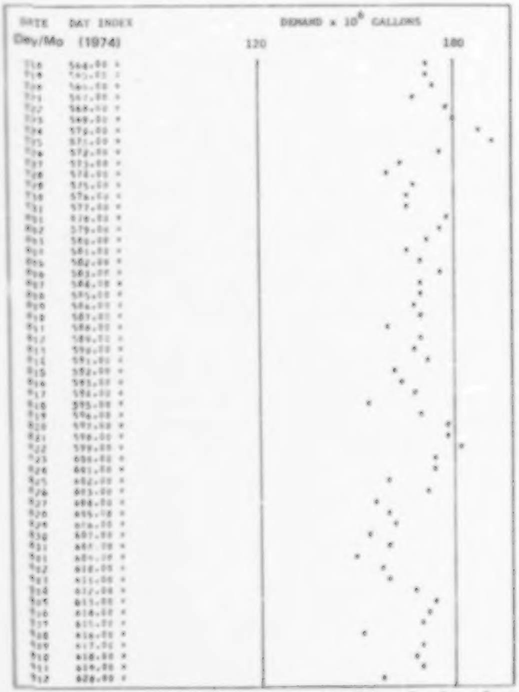

Figure 1. Example of Water Demand Time Series for Total System Demand for San Jose Water Works

It can also be assumed that

$$D(t) \sim N\left(B(t), \frac{\sigma^2}{1-a^2}\right) \qquad (5)$$

where

$$N\left(B(t), \frac{\sigma^2}{1-a^2}\right)$$

is a normal distribution with mean B(t) and variance

$$\frac{\sigma^2}{1-a^2}$$

Estimating and Updating the Base Element

The base effect can be modified by using short-run averages. This can best be formulated by introducing the notion of discounted estimation (discounted least squares). The problem is as follows:

Given D(t), $t = 0,\ldots,T$, it is required to estimate B(t)

where $$E[D(t)] = B(t) = \bar{B}_t \qquad (6)$$

$$Var[D(t)] = \frac{\sigma^2}{\beta^{T-t}}, \quad 0 < \beta < 1, \ \beta \text{ is known}, \quad t = 0, 1, \ldots, T \qquad (7)$$

where $\bar{B}_t$ is the true short-run average at t.

Equation (6) has replaced the time variability of the base by a constant and Equation (7) indicates that the variance on the demand gets larger the further back in time one goes (T is the present).

Using standard methods of estimating B, the result is:

$$\hat{B} = \frac{\sum_{i=0}^{T} \beta^{T-i} D(i)}{\sum_{i=0}^{T} \beta^{T-i}} \qquad (8)$$

Since

$$\sum_{i=0}^{T} \beta^{T-i} = \frac{1-\beta^{T+1}}{1-\beta} \qquad (9)$$

Then Equation (8) can be written in limiting form ($|\beta| < 1$, T large)and putting $1 - \beta = \alpha$) as:

$$\hat{B} = \sum_{i=0}^{T} \alpha \beta^i D(T-i) \qquad (10)$$

Writing $\hat{B}$ in Equation (10) as a function of t

$$\hat{B}(T) = \alpha D(T) + \sum_{i=1}^{T} \alpha \beta^i D(T-i) \qquad (11)$$

Equation (11) can be rewritten as

$$\hat{B}(T) = \alpha D(T) + \beta \hat{B}(T-1) \qquad (12)$$

Equation (12) is the key equation for estimating the base effect. The α is known as the "gain" of the estimates.

Equation (10) can be used to compute expectation and the variance of the estimator $\hat{B}(T)$.

$$E[\hat{B}(T)] = \sum_{i=0}^{T} \alpha \beta^i E[D(T-i)]$$

$$= \sum_{i=0}^{T} \alpha \beta^i \bar{B}_t = \bar{B}_T \qquad (13)$$

and $$Var(\hat{B}(T)) = \sigma^2 \qquad (14)$$

In summary, Equation (12) gives a procedure for updating the base. This equation is known as an exponential discount scheme. The gain is α and the discounting is $1 - \alpha$. To compute the effective memory of Equation (12), it is required to compare $(1-\alpha)^K$ with D(T) for various values of K. When $(1-\alpha)^K D(T)$ is relatively small, the effective memory is K time periods. The procedure is initialized by using

$$\bar{B}(T) = \frac{1}{T} \sum_{i=1}^{T} D(i) \qquad (15)$$

over an appropriate time period.

Estimating and Updating the Autoregressive Element

The autoregressive element of the model is estimated by forming

$$y_t \triangleq R(t) = D(t) - \hat{B}(t) \qquad (16)$$

over an appropriate part of the historical data base.

Using the Yule-Walker equations for an autoregressive process, the following result is obtained [4]:

$$\Gamma_0 \triangleq E\,[y_t y_t] = \frac{\sigma^2}{1-a^2} \qquad (17)$$

$$\Gamma_1 \triangleq E\,[y_t y_{t-1}] = \frac{-a\sigma^2}{(1-a^2)} \qquad (18)$$

Γ_0 and Γ_1 can be estimated by using either the maximum likelihood method or the method of moments [4,5].

The estimates are:

$$\hat{\Gamma}_0 = \frac{1}{N} \sum_{i=1}^{N} {y_i}^2 \qquad (19)$$

$$\hat{\Gamma}_1 = \frac{1}{N-1} \sum_{i=2}^{N} y_i y_{i-1} \qquad (20)$$

The same analysis that was carried out in the previous subsection can be implemented for the estimates of Γ_0 and Γ_1.

Letting γ be the gain, the result is:

$$\Gamma_0(N) = \gamma\, y^2_N + (1-\gamma)\, \hat{\Gamma}_0\, (N-1) \qquad (21)$$

$$\hat{\Gamma}_1(N) = \gamma\, y_N y_{N-1} + (1-\gamma)\, \hat{\Gamma}_1\, (N-1) \qquad (22)$$

The remarks in the previous subsection concerning the gain γ or the discounting factor $(1-\gamma)$ can be made here.

As in the previous subsection, the values of $\hat{\Gamma}_0$ and $\hat{\Gamma}_1$ are initialized by using Equations (19) and (20) over part of the historical data base.

Having estimates of $\hat{\Gamma}_0$ and $\hat{\Gamma}_1$, the estimate of a and σ^2 for the demand model is easily obtained using Equations (17) and (18) as follows:

$$\hat{a}(N) = \frac{-\Gamma_1(N)}{\Gamma_0(N)} \qquad (23)$$

$$\hat{\sigma}^2(N) = \Gamma_0(N)\,(1 - \hat{a}(N)^2) \qquad (24)$$

The Weather Model

An examination of a weather plot relating temperature to demand indicates that there exists a high degree of correlation between demand and incident temperatures. Figure 2 illustrates an example of such a scatter plot. The correlation coefficient for the data illustrated in Figure 2 is - 0.85. (Water demand increases with temperature.)

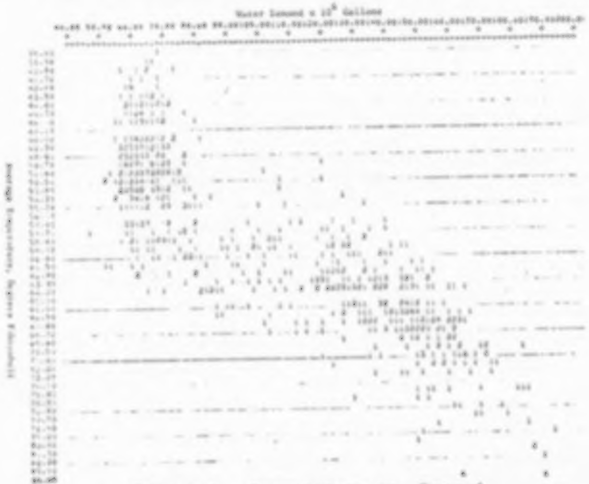

Figure 2. Temperature vs. Demand

Further examination of scatter plots for demand vs. temperature on the previous day indicates again that a strong correlation exists. This lagged correlation of course makes sense, since water demand is an effect that has "memory." Figure 3 illustrates the lagged temperature vs. demand correlation effect for the test data.

The fact that the lagged temperature vs. demand relationship is so strong, as well as the fact that when operating with a pure stochastic model the forecast "outliers" are highly weather-correlated, leads to the consideration of a structured weather model.

Before proceeding to a description of the model, a few remarks on the correlation of other weather variables with demand are in order. Scatter plots of other variables and demand are available in "Identification of Water Demand Models" [6].

An overview of the correlations of demand to lagged weather variables is presented in Figure 4 for the test data. From Figure 4, as well as the individual scatter plots, it becomes a clear that the only serious candidate for a set of exogenous variables are the lagged average temperatures.

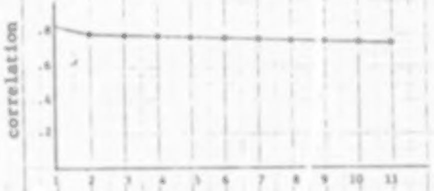

Figure 3. Lagged Days Average Temperature Correlated to Demand, 1973-1974, San Jose Water Works

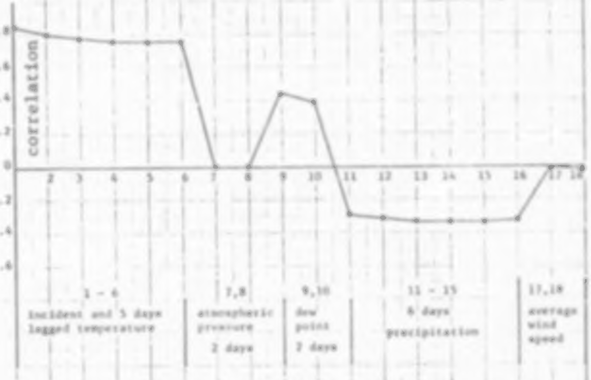

Figure 4. Lagged Days Other Weather Correlated to Demand, 1973, San Jose Water Works

In light of these introductory remarks on weather variables, the weather demand model is defined as follows:

$$D(t) = B(t) + W(t) + X(t) \qquad t = 0, 1, 2, \ldots \quad (25)$$

$$X(t) = b\, X(t-1) + u(t) \qquad t = 1, 2, \ldots \quad (26)$$

$$W(t) = c\, \Omega(t) \qquad t = 1, 2, \ldots \quad (27)$$

where

$D(t)$	is the water demand at time t
$B(t)$	is the base effect at time t
$W(t)$	is the weather component of demand given by Equation (27) where c is an unknown constant and $\Omega(t)$ is the effective weather variable at time t (defined later)
$X(t)$	is the autoregressive term given by Equation (26) where b is unknown and $u(t)$ is a sequence of independent random variables with $E[u(t)] = 0$ and $Var[u(t)] = \sigma^2$.

An examination of Equation (25) yields that the following parameters are to be estimated from the data base:

$B(t)$ = the base effect
c = the weather effect loading constant
b = the autoregressive coefficient
σ^2 = the model variance.

Observe that

$$E[D(t)] = B(t) + W(t) \tag{28}$$

and that

$$\mathrm{Var}\ D(t)/\ [W(t),\ B(t)] = \frac{\sigma^2}{1-b^2} \tag{29}$$

Equations (28) and (29) will be used for generating a weather demand forecast. Equation (29) means the conditional variance of $D(t)$ with respect to known $W(t)$ and $B(t)$.

As in the stochastic model, the parameters are estimated using step-wise regression. The mathematical details for the estimation of $B(t)$, b and σ^2, are similar to the details presented in the above section. The estimation c uses the same principles [6].

Identification of the Effective Weather Variable

The method of principal components (PC) is used to define an effective temperature [3,4]. The PC method works as follows:

Let $T_i' = (t_0, t_1, t_2, \ldots, t_k)$ be a vector of lagged temperature variables observed at time i (t_0 = incident temperature, t_j is lagged to day j temperature, etc.). Then the sample covariance matrix of the T_i' is defined as follows:

$$S = \frac{1}{n} \sum_{i=1}^{n} (T_i-\overline{T})\ (T_i-\overline{T})' \tag{30}$$

where

$$\overline{T} = \frac{1}{n} \sum_{i=1}^{n} T_i \tag{31}$$

Now suppose it is possible for an artibrary T vector to choose a set of vectors $C_1', C_2', \ldots, C_k'$ such that:

$$\mathrm{Var}(C_1'T) \geq \mathrm{Var}(C_2'T) \geq,\ \ldots,\ \geq (\mathrm{Var}(C_k'T) \tag{32}$$

and

$$C_i' \perp C_j' \qquad \text{for } i \neq j \text{ (orthogonal)} \tag{33}$$

and

$$||\ C_i'\ || = 1 \text{ (unit length)}$$

Then the quantities in (32) are called the principal components and the C_i, $i = 1, \ldots, k$ are called the principal component transformations. If it turns out that a small number of $\mathrm{Var}(C_i'T)$ explains most of the variance of S then these small number of scalar quantities can be used as effective (or substitute) independent variables in a regression problem. Further, it can be demonstrated that regression problems performed using principal components have smaller variance of the estimated coefficients than if the regression had been performed on the original untransformed variables [7].

For the test data of lagged temperatures (San Jose Water Works service area weather information 1973-1974), it turns out that 80% of the variability is explained by one variable.

The results for the principal component analysis are presented in Table 1. This table shows that one component is sufficient to define an effective weather variable.

Table 1

CORRELATION OF EFFECTIVE TEMPERATURE WITH DEMAND FOR 1973 AND 1974 SJWW DATA

COMPONENT YEAR	FIRST COMPONENT	SECOND COMPONENT
1973	Explains 79% of lagged temperature variance. Correlation = 0.87 95% Confidence = (0.84, 0.89)	Explains 8% of lagged temperature variance. Correlation = -0.10 95% Confidence = (-0.20, 0.00)
1974	Explains 83% of lagged temperature variance. Correlation = 0.86 95% Confidence = (0.83, 0.88)	Explains 7% of lagged temperature variance. Correlation = -0.14 95% Confidence = (-0.23, 0.00)

Performance of Models for San Jose Data

A summary of the data analysis is as follows:

1. The weather model and the stochastic model are completely correlated for one-step-ahead forecasting.
2. The best stochastic model performance is given in Table 2 for a data base of 682 days through all seasons of a year.

Table 2

OVERVIEW OF PERFORMANCE OF STOCHASTIC MODEL FOR APPROXIMATELY TWO YEARS OF FORECASTING

R = Relative Error in %	% of Days With Error Less Than R
3.5	40
7.0	62
10.5	78

Details on the performance will be provided in Figures 5 - 8. Complete details are available in [6].

Figure 5 illustrates the distribution of the relative errors for the choice of *a priori* parameters $\alpha = 0.8$ and $\gamma = 0.8$. From this figure it is clear that most of the relative errors are less than 7%.

Figure 6 presents a histogram of the forecast standard deviations for $\alpha = 0.8$ and $\gamma = 0.8$. Figure 7 illustrates the number of estimated standard deviations that the actual value of demand differs from the forecast demand.

The utility of Figures 6 and 7 becomes apparent when probabilistic forecasts are made using the forecasted standard deviation. For example, suppose the forecasted demand is $\hat{D}$ and that the forecasted standard deviation is $\hat{\sigma}$. Then Figure 7 is used to construct the probability associated with the confidence interval for the true demand, D, as follows:

$$\hat{D} \pm 2.27\ \hat{\sigma} = 55\%\ \text{confidence for true demand}$$

and

$$\hat{D} \pm 6.80\ \hat{\sigma} = 78\%\ \text{confidence for true demand}$$

That is to say, $\hat{D} \pm 2.27\ \hat{\sigma}$ contains the true demand with 55% probability.

From Figure 5 it can be observed that a value of $\hat{\sigma} = 1 \times 10^6$ is "typical." Therefore, in a "typical" case, demand can be forecasted to roughly 2.3×10^6 gallons.

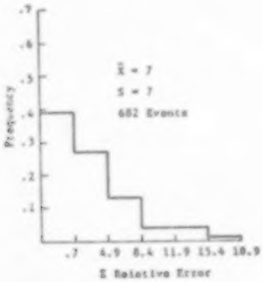

Figure 5. Distribution of Stochastic Residuals ($\alpha = .8$, $\gamma = .8$)

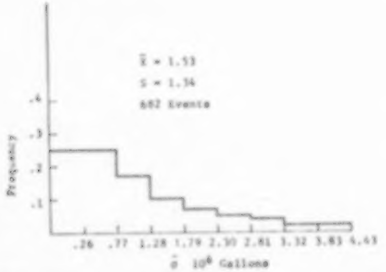

Figure 6. Distribution of $\hat{\sigma}$ for Stochastic Model ($\alpha = .8$, $\gamma = .8$)

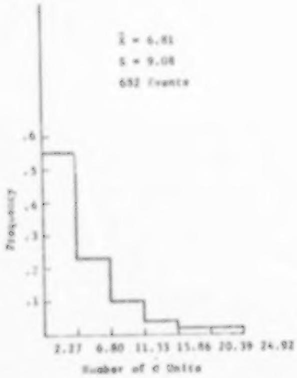

Figure 7. Number of $\hat{\sigma}$ Units Forecast Deviates from Actual ($\alpha = .8$, $\gamma = .8$)

It is important to note that the 75% confidence interval can be used to "flag" outliers or anomalies in the forecast.

Figure 8 shows the distribution of the estimated parameter $\hat{a}$ for the stochastic model. Recall that $\hat{a}$ is the autoregressive loading for the model. Values of $\hat{a} > 1$ imply that the model is becoming unstable.

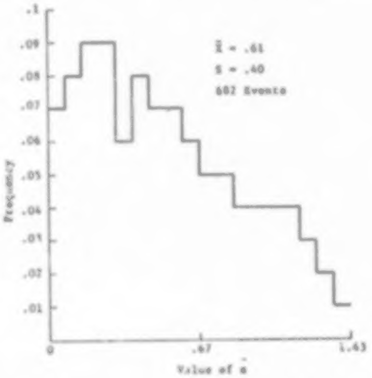

Figure 8. Distribution of the Estimated Parameter $\hat{a}$

Acknowledgement

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HYDROLOGIC IMPACT STUDIES OF ALTERNATIVES TO MEET WATER NEEDS IN SOUTH-CENTRAL PENNSYLVANIA

David H. Marks, Guillermo J. Vicens, Brendan M. Harley, and John C. Schaake, Jr.[1]
Resource Analysis, Inc., 1050 Massachusetts Avenue, Cambridge, Massachusetts 02138

ABSTRACT

This paper presents the use of several interrelated models to investigate the potential hydrologic impacts of several proposed water supply alternatives for the South Central Pennsylvania area. The area contains major demand centers in Harrisburg,York, Lancaster, Lebanon, Manheim, Elizabethtown, Ephrata, New Holland, Lititz, Carlisle, and Mechanicsburg, which for the most part depend on local surface waters for their water supply with supplemental withdrawals from the Susquehanna River and from groundwater. Withdrawals from all of these sources could have an impact on the flows in the Susquehanna itself. Since this river is the main source of freshwater to Chesapeake Bay, it was important to assess the relative impact of each of the proposed alternatives on the outflow distribution to the Bay. The scope of the study was limited to the hydrologic aspects of the problem. The models used to evaluate the impacts of the alternatives were:

1. A synthetic streamflow augmentation and generation model to first augment the existing records up to a full 80-years, and second generate a set of 200-year synthetic records which resembled the historical records in their statistics.

2. A linear regression model relating monthly rainfall and evapotranspiration to streamflow in the tributaries used to evaluate the impact of groundwater withdrawals on surface water flows.

3. A simulation model used as an accounting device to show the impact of the alternatives on the monthly flows at several locations in the area including the outflow of the Susquehanna to Chesapeake Bay.

INTRODUCTION

The objective of this paper is to describe the methodology used in hydrologic investigations carried out on a series of water supply alternatives for the South Central Pennsylvania area (Resource Analysis, Inc., 1974b). The area contains major demand centers in Harrisburg, York, Lancaster, Lebanon, Manheim, Elizabethtown, Ephrata, New Holland, Lititz, Carlisle and Mechanicsburg, Pennsylvania as shown in Figure 1. In general, these communities depend on local surface water for their water supplies, with additional supplies coming from the Susquehanna River and from groundwater. With continuing increases in population in the area, major capital investment in new facilities and water sources will be necessary. Withdrawals from groundwater or local surface water storage may have a different impact on flows in the Susquehanna and its tributaries than withdrawals from the Susquehanna itself. While the area is itself relatively water rich, different withdrawal patterns will lead to changes in the flow characteristics of the local tributaries and to different distributions of outflows from the Susquehanna to Chesapeake Bay. Since a change in the outflow distribution for the main freshwater input to the Bay could have major ecological impacts, this outflow is of significant interest.

Objectives of Study

The primary objective of the study was to assess the relative impact of the proposed alternatives for water supply development on the distribution of monthly outflows from the study area. In addition, estimates of the impacts on low flows in local tributaries were made. Other parts of the study conducted by other contractors dealt with institutional, ecologic, and engineering feasibility considerations. Our study dealt only with hydrologic considerations, i.e., the distribution of outflows from the system and on the tributaries as they are affected by the different alternatives.

Study Area

The study area is shown in Figure 1 and contains all or parts of Cumberland, Adams, York, Dauphin, Lebanon, and Lancaster Counties in the south central part of the Commonwealth of Pennsylvania. Major tributaries to the Susquehanna River in the study area are Swatara, East Conewago, Chickies, and Conestoga Creeks on the east side; and Conodoquinet, Yellow Breeches, West Conewago, and Codorus Creeks on the west side. Present water supply usage and future water demand (year 2020) are shown for each major municipal area in Table 1. The major demand areas include surrounding water companies as well as the new municipalities. In general, Harrisburg (East) presently depends on Clark, Stony, and Swatara Creek sources; Harrisburg (West) on Yellow Breeches, and Conodoquinet Creeks; Mechanicsburg on Yellow Breeches; Elizabethtown and Manheim on Chickies Creek; Lebanon on the Swatara; Lititz and New Holland on groundwater; Ephrata on Conestoga Creek; and York on the Codorus. Only Lancaster presently draws major supplies from the Susquehanna.

Alternatives for Water Supply

A variety of different water supply options exists for the area ranging from all ground and local surface water to all Susquehanna water, as well as combinations of the two. As there is a relatively large amount of water available in the area, the question of importance is which sources should be developed rather than whether it is possible to find the water. For example, Harrisburg (East and West), Mechanicsburg, Lebanon, Elizabethtown, York, Lancaster, and New Holland could go directly to the Susquehanna for additional sources. Alternatively, new or improved impoundments on the Conodoquinet, Swatara, E. Conewago, and W. Conewago Creeks; and the South Branch of Codorus Creek could also be used to supply future water needs. Groundwater in areas like York, Lebanon, Elizabethtown, Ephrata and New Holland could serve their new water needs. To consider the options available a series of alternatives were conceived by the U.S. Army Corps of Engineers and the Commonwealth of Pennsylvania, and developed by the Anderson-Nichols Co. to consider combinations of these possibilities. A brief discussion of the alternatives is shown in Appendix A.

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[1] Now at Hydrologic Research Laboratory, National Weather Service, Silver Spring, Maryland 20910

Water Supply Service Areas and Demands for 1970 and 2020

Table 1

Major Demand Areas	Municipalities Included	Demand (MGD) 1970	Demand (MGD) 2020
Carlisle	Carlisle Boro and Suburban	3.7	6.9
Mechanicsburg	Millsburg, Grantham, Mechanicsburg W.C.	1.8	6.2
Harrisburg (West)	Riverton W.C.	7.7	19.8
Harrisburg (East)	Harrisburg W.C., Dauphin, Hershey, Middletown, Steeltown	22.4	32.7
Lebanon	Lebanon City, Keystone, Cornwall, Meyerstown, Heidelburg	8.2	16.8
York	Red Lion, Dover Boro, Dover Twp., West Manchester, York W.C.	21.0	40.2
Elizabethtown	Rheems, Elizabethtown, Mount Jay	0.8	3.6
Manheim	Manheim	0.5	0.7
Lancaster	Columbia, Mountville, E. Hempstead, E. Petersburg, Lancaster, Millers	17.4	40.1
Lititz	Lititz	1.0	3.0
Ephrata	Akron, W. Earlham, Ephrata	1.1	2.2
New Holland	Leola, New Holland, Blue Bell	0.7	2.7
Total		86.3	174.9

Outline of Methodology

The information available for this study was the following:

1. Estimates of future demands from municipal and industrial (M&I), agricultural, and consumptive powers cooling users.
2. Monthly gauging records for several locations in the area including the Susquehanna River, Codorus, Conodoquinet, Swatara, W. Conewego, and Conestoga Creeks.
3. Monthly precipitation records at York, Harrisburg, Lancaster, and Lebanon.
4. Configurations for each water supply alternative including reservoir capacities and allocation of demands to sources.

Given this data base, the objective was to assess the hydrologic impacts of each alternative through a simulation study. The following tasks were carried out to evaluate the alternatives:

1. Process the rainfall and streamflow data into the RAI Hydrologic Data Management System (Resource Analysis, Inc., 1974a).
2. Augment the streamflow records to produce a "full" set of records of consistent length to be used for parameter estimation purposes.
3. Estimate the statistical parameters of these records, and generate a set of 200-year synthetic records.
4. Develop a linear regression model relating the effect of groundwater withdrawal on future streamflows. This relation was to be used to assess impacts of groundwater development on local surface water flows.
5. Simulate the operation of the system under both the historical and synthetic streamflow records for each alternative plan in order to assess its reliability and the resulting hydrologic impacts.

The following sections briefly describe each of the above steps. A full discussion of the methodology and results is contained in the final project report, Resource Analysis, Inc. (1974b).

GENERATION OF SYNTHETIC STREAMFLOW RECORDS

Available Streamflow Data

Historical records at eleven gauging sites in or near the study area were available. The length of these records is shown on Figure 2. All stations had at least 40 years of observations except for Station 5755 which had 32 years, and Stations 5745 and 5765 which had some small gaps.

An improvement in the parameter estimates was obtained by extending or "filling-in" the shorter records by correlation with nearby stations. Regression analysis has been frequently used to carry out the augmentation of records. The theory on which these procedures are based has been discussed by Fiering (1962), Matalas and Jacobs (1964), and Gilroy (1970), and will only be briefly summarized here.

The streamflow data at the gauging stations with the shorter record y_t, are related to the data at other sites $x_{1t}, x_{2t}, \ldots, x_{pt}$, through a linear regression model given by:

$$y_t = a + b_1 x_{1t} + b_2 x_{2t} + \ldots + b_p x_{pt} + e_t \qquad (1)$$

where e_t is a standardized normal random deviate. The parameters of this model $a, b_1, b_2, \ldots,$ and b_p are computed from the available data through standard least square procedures for regression analysis. These values are then used in the model to estimate the streamflow at station y where these values are missing. Similarly, in the case of shorter records, the record at station y is extended by this same procedure from the longer observed nearby or related records.

Three data augmentation runs were carried out. These are described in Table 2. The objective of the first run was to obtain a full forty years. Run No. 2 extended the 8 stations to 73 years. Finally in Run No. 3, the nine shorter records were extended an additional seven years by regression from the longest record. The final output was a set of 80-year records at all eleven stations.

Table 2

Data Augmentation

Run No.	Stations Augmented	Other Stations	Period Augmented	Period of Estimation
1	5145 5755 5765	5730 5705 5700 5750 5740	10/1932 to 9/1972	*10/1932 to 9/1972
2	5700 5730 5745 5750 5760 5765 5740 5755	5670 5705	10/1899 to 9/1972	10/1932 to 9/1968
3	5670 5700 5745 5750 5760 5765 5730 5255	5705	10/1891 to 9/1972	10/1932 to 9/1968

*Includes only extension of record length, not monthly gaps.

Synthetic Streamflow Generation

A 200-year synthetic streamflow record was generated based on the procedures described in Valencia and Schaake (1972, 1973). Briefly, the procedure is first to generate a series of annual flows at the selected stations. These annual flows are then disaggregated into seasonal flows. Finally, a similar procedure disaggregates seasonal flows into monthly flows. This scheme preserves the means and variances of the seasonal and monthly flows, the correlation between monthly flows at the same site or different sites, and the correlation between any monthly flow and any seasonal flow and between the seasonal flow and the annual flow. The generated monthly values at any site will add up to the corresponding annual value, which guarantees the preservation of annual statistics.

GROUNDWATER MODEL

A simple model of the impacts of groundwater withdrawals on surface water flows was developed. This model was based on a theoretical analysis of the range of potential impacts to be expected, as well as a statistical analysis of rainfall and streamflow data to evaluate the dynamic properties of the aquifers in the study region.

The historical rainfall and streamflow records available for this region were used to determine the time delay characteristics of the natural groundwater system. A mathematical description of this system was created, based on the following assumptions. First, the average streamflow in each month consists of groundwater and direct runoff components. Second, the amount of direct runoff is assumed to depend upon the current month's precipitation. Finally, the amount of groundwater is assumed to depend upon the current and previous months' precipitation in excess of evapotranspiration. An equation representing this is:

$$Q_t = a_0 + a_1 P_t + \sum_{i=0}^{6} b_i \left(P_{t-i} - E_{t-i}\right) + V_t \qquad (2)$$

where Q_t represents streamflow in month t, P_t and E_t denote the rainfall and evapotranspiration in month t, and the values of a_0, a_1, b_0, ... , b_m are to be evaluated for each sub-basin. The precipitation variables P_t should be basin average values which can only be estimated from point values. Likewise, the evapotranspiration variable, E_t, should be the basin average value. The disturbance term V_t accounts for the errors introduced by using point measurements instead of the "true" basin average values.

The effects of groundwater withdrawals on surface flows was then assumed to be similar in response to the rainfall-runoff relations derived above. Thus the streamflow depletion in month t denoted as D_t was related to the groundwater withdrawals for the six previous months, W_t through W_{t-6}, by:

$$D_t = \sum_{i=0}^{6} c_i W_{t-i} \qquad (3)$$

where the coefficients C_i are computed from:

$$c_i = \frac{b_i}{\sum_{i=0}^{6} b_i} \qquad (4)$$

A similar formulation was used by Nieswand and Granstrom (1971) to model the Mullica River Basin in New Jersey.

The coefficients obtained from the analysis of the Susquehanna data are shown in Table 3.

Table 3

Groundwater Withdrawal Impacts on Local Streamflows

BASIN	Streamflow responses in various months due to a unit groundwater withdrawal in month t						
	t	t+1	t+2	t+3	t+4	t+5	t+6
Codorus Creek	.147	.188	.237	.212	.151	.051	.014
Conodoquinet Creek	.178	.171	.225	.201	.153	.018	.054
Swatara Creek	.456	.207	.105	.087	.115	.030	0.00
Conestoga Creek	.165	.139	.175	.206	.165	.102	.048

SIMULATION MODEL

To assess the impacts of each of the alternatives on the distribution of flows in the Susquehanna and the low flows in the tributaries, and to evaluate the reliability of the proposed alternatives, a simulation study of the operation of the system was carried out. A modified version of the MIT River Basin SIMulation

Model (MITSIM) was used for this purpose (Schaake, et. al, 1974).

MITSIM was designed to generate and display both economic and physical information to aid in evaluating system response. The model is an accounting procedure that takes the synthetic or historical data developed, seasonal water demands and consumptive use, the groundwater response functions, the operating rules for the various reservoirs, pipelines, and groundwater systems, and operates them to find the monthly system flows at specified locations. The structure of the model is of nodes connected by branches with all water entering or leaving the system at the nodes. Typical nodes are:

1. Start nodes - nodes at which historic or synthetic streamflow data is input to the system. For the case study, a start node was used for all streams including non-gauged streams, and major overland flow areas to the Susquehanna. A special program was written to disaggregate data available at gauging stations (both historic and synthetic records) to input data for the start nodes.

2. Confluence nodes - the joining of two branches of the system used to show the connectivity of the activities.

3. Reservoir nodes - for each reservoir node, a capacity, seasonal target, and seasonal release schedule is given. Water may be removed from a reservoir node to meet demands provided enough water is in storage and release requirements are met.

4. Groundwater Nodes - represents the pumping of groundwater to meet a specified demand. A groundwater function relates seasonal withdrawal to impacts on local surface water in present and future seasonal withdrawal to impacts on local surface water in present and future seasons. A seasonal consumptive use coefficient shows how much of the groundwater is released to the surface water after use.

5. Irrigation Node - for each irrigation area, seasonal demands and consumptive use coefficients are combined to compute the portion of the specified demand in season that is returned to local surface waters in the present and future seasons.

6. M&I Node - a municipal and industrial demand and consumptive use coefficient is specified for each surface water demand in each season to calculate withdrawals and returns to streams.

   A typical schematic for a system is shown in Figure 3 and Appendix B describes the function of each of the nodes shown.

RESULTS

All of the alternatives described in Appendix A were simulated with the 200-year synthetic record. In addition, Alternatives 1,2 and 3 were simulated with the 80-year augmented historical record as inputs. The first question to be investigated was which of the records was more stringent or conservative. Comparison of the simulation results of Alternatives 1 through 3 for both the historic and synthetic records, showed that the 200-year synthetic record produced, on the average, lower monthly outflows from the study area even though two extensive drought periods were observed in the historic record. Since the relative impact of the alternatives on the distribution of the outflows from the system was of utmost importance in this study, the synthetic record was selected for detailed comparison of alternatives.

Monthly outflows were calculated at the lower boundary of the study area which was the intersection of the boundary of Lancaster County, Pennsylvania with the Susquehanna River. This line is slightly above the Conowingo pool, and thus our calculation of system outflow represents runoff from a slightly smaller drainage area than that supporting inflows to the Conowingo Pool, which other studies have focused on.

Table 4 presents a summary of the results obtained from the simulation runs. This table shows estimates of the annual and monthly 30-day low flow which occurs, on the average, once every twenty years (Q30-20) at the outflow of the study area. The results for each alternative plan with Year 2020 demands are shown, as well as a "Present" case for comparison purposes.

Table 4

Estimates of Q30-20 at the System Outflow 200-Year Synthetic Streamflow Trace and 2020 Demands. (Present Run Uses 200-Year Synthetic Trace and 1970 Data).

		Q30-20 (cfs)		
Altern.	Aug.	Sept.	Oct.	Annual
Present	3622	3266	3055	3075
1	3412	3051	2943	2840
2	3410	3050	2945	2820
3	3405	3048	2944	2818
4	3411	3052	2944	2840
5A	3411	3052	2944	2840
5B	3411	3052	2944	2840
5C	3405	3048	2944	2818
6A	3415	3056	2944	2853
6B	3425	3044	2944	2873
6C	3411	3052	2944	2840
7A	3422	3062	2946	2858
7B	3427	3065	2945	2879
7C	3407	3050	2945	2821

The overall results of the study were:

1. There is very little difference between alternatives in terms of Q30-20 or monthly average flows at the outflow of the study area. The values of annual Q30-20 for the alternatives range from 2818 cfs to 2879 cfs. The present case produces a value of 3075 cfs. Estimates of Q30-20 for August, September and October show similar results. Most of this decrease is due to a consumptive use increase in power cooling through 2020, which peaks at 345 cfs. The lower values are also due to increased groundwater and Susquehanna water usage, while the higher values are a result of reservoir storage in the tributaries.

2. From the viewpoint of flows in the tributaries, the alternatives with large groundwater usage decrease tributary flows slightly. However, all other alternatives tend to substantially increase tributary flows due either to diversions of Susquehanna water or larger reservoir impoundments.

3. Any reliability problems for M&I water availability are due to over estimates of present source capabilities and can be easily improved by increasing reliance on new sources. All alternatives are equally reliable.

SUMMARY

The use of several interrelated models to investigate the potential hydrologic impacts of several proposed water supply alternatives for South Central Pennsylvania has been presented. The objective of the study was to assess the relative impacts of the alternatives on the distrubution of the outflows to Chesapeake Bay. The methodology developed for this study consisted of several hydrologic models which processed the available hydrologic and water demand data to evaluate the impacts of the alternatives.

ACKNOWLEDGEMENTS

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Appendix A

DESCRIPTION OF ALTERNATIVES

Alternative #	Developments
1	Considers development each municipality would undertake without outside assistance. Harrisburg, Mechanicsburg, and Carlisle would draw from present sources with some additional groundwater development. Lebanon would develop new storage and improve existing storage on the Swatara, with some new groundwater development. York would go to the Susquehanna as a source and develop groundwater. Elizabethtown, Ephrata, New Holland, and Lititz would develop additional groundwater sources. Lancaster and Manheim would continue with present sources.
2	Considers major use of groundwater in the future, especially for York and Lebanon. No new impoundments or Susquehanna sources.
3	Considers Susquehanna as the major source of new water demands for Lebanon, York, and Elizabethtown, with no new impoundments built.
4	Considers new impoundment on Swatara Creek for Lebanon, and York water supply from Susquehanna.
5A	Considers impoundment on Swatara Creek for Lebanon and Elizabethtown, and York supply from Susquehanna.
5B	Same as 5A except reservoir development on E. Conewago Creek is considered for Elizabethtown.
5C	Susquehanna is used for Lebanon, Harrisburg, (East and West), York and for some additional needs in Carlisle and Mechanicsburg. Reservoir on E. Conewago Creek is used for Elizabethtown.
6A	Considers a new reservoir on the Swatara and groundwater for Lebanon. New reservoir on S. Branch of the Codorus for York.
6B	Lebanon impoundment retained, but Elizabethtown switched to Susquehanna and York to a W. Conewago reservoir.
6C	York, Lancaster, New Holland and Elizabethtown use Susquehanna, and new impoundments are developed on Conodoquinet Creek and Swatara Creek.
7A	Large groundwater development, Lebanon uses Susquehanna and York uses impoundment on W. Conewago Creek.
7B	Same as 7A except Lebanon uses a reservoir on the Swatara.
7C	Combines 5C and 6C and includes a reservoir on the Conodoquinet.

Appendix B Node Descriptions

Reservoir - CODRRES
M&I - CARLILMI, HARRWCDQ, MECHBGMI, HARRWYBC, YORKCODR, YORKCBC, YORKSUSQ, LANCSTSQ, EPHRTAMI, ELIZCHK, MANHMMI, LEBSWT, HARRESWT, HESUSQ, HARRESCL, SUSQMI
Groundwater - CARLILGW, MECHBGGW, YORKGW, LEBANGW, ELIZGW, LITITZGW, NEWHOLGW, LANCSTGW, EPHRTAGW
Irrigation - CDQIRR, WCONIRR, CODRIRR, CSTIRR, CONWIRR, SWTIRR

All others are start or confluence nodes.

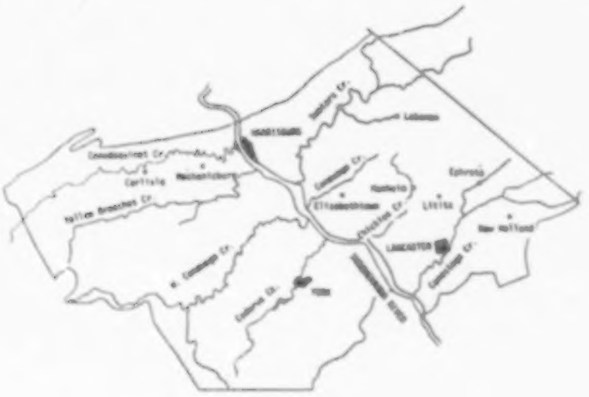
Conodoguinet Cr.
Carlisle
Mechanicsburg
HARRISBURG
Swatara Cr.
Lebanon
Yellow Breeches Cr.
Conewago Cr.
Manheim
Elizabethtown
Ephrata
Lititz
Chickies Cr.
New Holland
LANCASTER
Conestoga Cr.
W. Conewago Cr.
Codorus Cr.
YORK
SUSQUEHANNA RIVER

Figure 1: Study Area

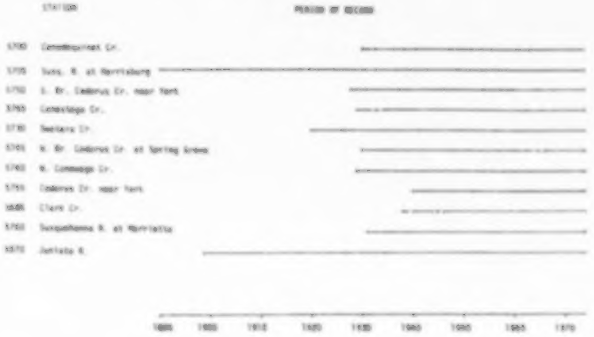

Figure 2: Available Streamflow Records

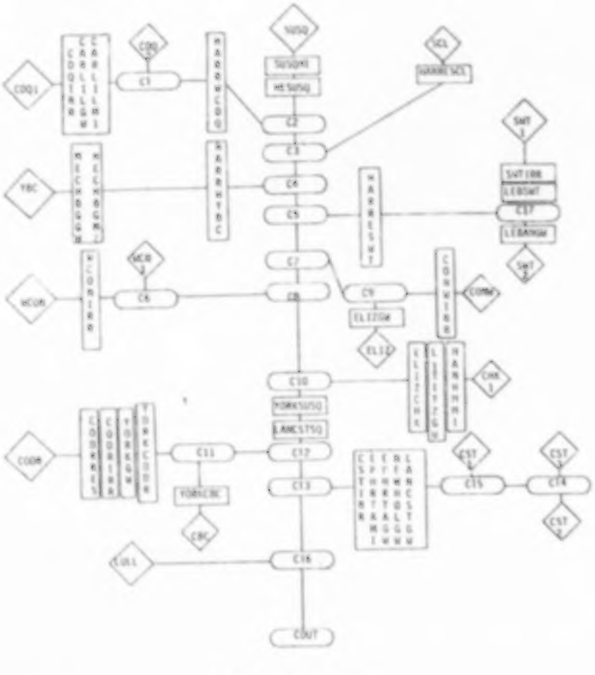
SUSQ
CDQ
SCL
CDQ1
C1
SUSQMI
HESUSQ
HARRESCL
C2
C3
SWT 1
SWT100
LEBSWT
C17
LEBANGW
SWT 2
YBC
C4
C5
WCON
C6
C7
C8
C9
ELIZGW
ELIZ
C10
CHK 1
YORKSUSQ
LANCSTSQ
CODR
C11
C12
C13
YORKCBC
CBC
CST
C15
C14
CST 2
C16
COUT

Figure 3: Typical Schematic

THE OPERATIONAL WATER QUANTITY MODEL

Ashok N. Shahane
Environmental Systems Engineer

Paul Berger
Scientific Programmer

Robert L. Hamrick
Division Director

Water Planning Division, Resource Planning Department
Central and Southern Florida Flood Control District
West Palm Beach, Florida 33402

SUMMARY

A recently completed operational water quantity model based on hydrologic-hydraulic simulations is presented in this paper. Using the rainfall input, initial state conditions and basin parameters, the model estimates, among many hydrologic entities, the streamflows contributed by the watersheds. An iterative type routing model is then developed to distribute the simulated streamflows through the primary conveyance systems of lakes, canals, and channelized river controlled by the gate operations at the controlling structures. The designed methodology is demonstrated for the Kissimmee River basin of Florida for the year 1970 by considering 21 canals, 14 lakes and 14 controlling structures. The outcome of the model relates to simulated lake stages, water levels at tailwater and headwater sides of the controlling structures and simulated discharges through controlling structures every 3 hours for the full year of 1970. The comparison of simulated values with the corresponding historical data indicates clearly the "working" of all the individual pieces of the operational water quantity model, although a few critical links are currently being refined to obtain better simulated lake stages.

INTRODUCTION

Although the conventional watershed models are developed with different purposes, methodologies, tools and settings, they are usually valid for natural hydrologic drainage systems. Therefore, it seems that these models have to be modified in some fashion to analyze the typical water system with a chain of lakes and channels managed by several controlling structures. Thus, a basic characteristic of the operational water quantity model is related to its capability of including operational functions of the water system with adequate theoretical and experimental data for formulating basic hydrologic processes. Secondly, based on the analytical principles, simulation and optimization techniques with stochastic and deterministic inputs are currently being used in planning and design of water systems. Considering the necessary assumptions and speculated conditions required for reaching a mathematical solution, these design models give general answers to the overall problem and do not generate the most desired product for the operational needs[4]: As further pointed out by Lindahl and Hamrick[4], operationally oriented models should give specific answers to very specific questions and circumstances. Thirdly, the operational models are usually designed to function as a short-term and long-term decision making aide within an operational set-up and within existing peripherial monitoring capabilities for a typical system. In other words, using hydrologic and hydraulic characteristics of the river basin, the operational models can provide valuable assistance in operating the gates manually or automatically to maintain water levels or adequate flow of water in normal as well as unusual circumstances.

The specific water system for which the presented operational water quantity model was developed is the Kissimmee River system as depicted in Figure 1. As shown in Figure 1, the Kissimmee water system consists of 14 lakes, 25 canals and 14 controlling structures. As shown in Figure 2, the Kissimmee basin is further divided into 19 drainage basins (also called planning units) that drain into the primary conveyance system of lakes, canals and controlling structures of Figure 1. It is to be emphasized that the procedure of the operational water quantity model and the related computer programs are developed for specific configuration of the water system as shown in Figures 1 and 2.

COMPONENTS OF THE OPERATIONAL WATER QUANTITY MODEL

Since past attempts have been made in three distinct stages to bring the model to its current form, its developmental procedure is broken down into three component parts: 1. Sub-basin model, 2. Routing procedure, and 3. Routing methodology to combine the routing technique with the sub-basin model. Basic computational steps of the model are outlined in Figure 3.

Description of the sub-basin model:

The basic foundation on which the sub-basin model was developed and modified is essentially a parametric approach for formulating the physical system of the Kissimmee basin in terms of hydrologic simulation.[4,5,8,9,10] It can be seen from Figure 4 that the major computational steps are related to: (a) processing of input rainfall values, (b) Formulations of infiltration phenomenon, (c) surface storage and overland flow equations, (d) estimation of water losses, and (e) quantification and routing of subsurface flow through a multi-layer soil system.

Since the detailed descriptions and discussions of rationale behind these formulations were previously reported by Holtan, Lopez, Lindahl, Sinha, Hamrick, Khanal, and Shahane, et. al,[1,2,4,5,8,9,10] these formulations are briefly discussed in the following section.

Processing of input rainfall values: Using the available network of raingaging stations over the entire Kissimmee River basin, daily rainfall values are obtained for each of the 19 planning units from the daily rainfall values of surrounding representative raingaging stations. These recorded daily rainfall values are further synthesized to generate hourly values using a linear stochastic model for the consecutive hourly rainfall record as reported in reference 10.

Formulations for infiltration phenomenon: Among various formulations and concepts proposed by many soil scientists, a modified form of the empirical equations originally developed by Holtan is used in quantifying the infiltration phenomenon.[1,2] Such equations are:

$$f = A(SA)^{1.4} \text{ for } SA \geq G \text{ - - - - - - - - - - - } (1)$$

and

$$f = A(SA)^{1.4} + FC \text{ for } SA < G \text{ - - - - - - - - } (2)$$

where

f = capacity rate of filtration, A = surface penetration index, SA = storage currently available in the soil reservoir, FC = constant rate of infiltration between consecutive layers, G = total amount of free or gravitational water in a soil profile of selected depth.[1,2,8,9]

Surface storage and overland flow: Besides infiltration, a part of precipitation is contributed to the storage in surface depressions. Such surface storage is computed as

$$VD = P - f \cdot DT \text{ - - - - - - - - - - - - - - - } (3)$$

After a part of precipitation input percolated into the ground and after a part filled the maximum volume of surface depressions, precipitation excess is contributed to overland flow. Mathematically, it is computed from simple subtraction as

$$\text{Overland flow} = P - f \text{ when } VD = VDM \text{ and } P > f \quad (4)$$

where

P = precipitation input, f = infiltration rate, VD = amount of water currently stored in surface depressions, VDM = maximum volume of surface storage.[8,9]

Estimation of water losses: In the sub-basin model, water losses are considered as the part of precipitation input that reaches the ground surface but never appears at the watershed outlet.[4,8,9,10] With this definition, water loss can occur in different categories; i.e., water loss due to direct soil evaporation, evapotranspiration by existing vegetation and water loss due to deep percolation. These losses are in turn functions of various factors as shown in the following formulations:

1. Water loss due to indirect soil evaporation,

$$\text{Loss 1} = C_1\left(1 - \frac{DWT}{DWTM}\right)\left[\frac{EP(NW)}{24}\right](DT) \text{ - - - - - } (5)$$

2. Portion of water that is lost due primarily to the existing vegetation

$$\text{Loss 2} = C_2(G_1)\left[\frac{EP(NW)}{24}\right] DT \text{ - - - - - - - - - } (6)$$

3. Water loss due to deep percolation,

$$\text{Loss 3} = (FC)(DT) \text{ - - - - - - - - - - - - } (7)$$

where

C_1 = ratio of maximum evapotranspiration to maximum pan evaporation value,
DWT = water table depth = (SA)(D)/G; - - - - - (8)
D = total depth of soil profile, G = total amount of free gravity water that could exist in a soil profile, DWTM = maximum depth to water table at which DWT will have a negligible contribution toward Loss 1, EP = pan evaporation, NW = number of weeks, DT = time increment, C_2 = constant = 0.78, G_1 = an overall growth index for the existing vegetation, FC = constant rate of infiltration between consecutive layers, SA = storage currently available in reservoir.

Adding these three losses together gives the total loss of water from a given soil profile. This value of total water loss is accounted for in estimating the recovery of water from the soil reservoir to the main channel.

Quantification and routing of sub-surface flow: The basic purpose of this computational step is to estimate the spatial and time contribution of the sub-basin flow from different soil reservoirs to the main channel. Thus, the first task is to determine the number of reservoirs. This is done by reverse integration of the runoff hydrograph by establishing storage-flow relationships for a simple recession curve. Using this technique it is established that for our 19 planning units, soil profile can be represented by not more than three soil reservoirs. After determining the number of soil reservoirs, the basic continuity equation and a storage outflow curve is combined to provide contributions of each soil reservoir to the stream channel and also the total storage available in these reservoirs at the end of each time step. These computations reported by Lindahl[4] take into account (1)the volume of water that is infiltrated during time DT, (2)initial available storage in a soil reservoir, (3)sum of water losses, (4)volume of subsurface drainable water, (5)time interval for the volume of the subsurface drainable water, and (6)the updated available storage. At the end of these computations, the discharges contributed by each soil layer and overland flow are obtained for each time interval. In the next step, these discharges are multiplied by the routing coefficients (which are estimated from Nash's routing equation) and resulting values are added together to obtain time distribution of streamflows at the watershed outlet.[8,9]

Input Data Requirements:

To carry out these computational steps for the 19 planning units of the Kissimmee basin, the parameters of the formulations should be known. Since these parameters represent the agricultural-related water characteristics of the basin, they are estimated based on the available research publications of the ARS and many reports delineating the regional characteristics.[4,5,8,9,10]

To compute infiltration characteristics, the appropriate basin parameters are: (a) total available storage in three soil reservoirs, i.e., TAS(1), TAS(2) and TAS(3); (b) constant rates of infiltration in three layered soil systems from one layer to another designated as F(1), F(2) and F(3); (c) total ammount of gravitational water in these three layers, i.e., G(1), G(2), and G(3); (d) portion of G that can be drawn into surface water i.e., GD(1), GD(2), and GD(3),and (e) total depth of the soil profile (D) in inches.

In addition, for estimating three types of water losses, overland flow, and sub-surface flow, the following parameters are required: (a) depth of water table at which evaporative water loss is considered significant, (b) maximum volume of surface storage (VDM), (c) ratio of evapotranspiration and maximum pan evaporation value (PPAN), (d) sub-surface discharges through three soil layers Q(1), Q(2), and Q(3), and (e) corresponding storages in these three soil reservoirs SG(1), SG(2), and SG(3).

Finally, routing coefficients to combine flows from three sub-surface layers with the overland flow i.e., TK(1), TK(2), TK(3), TK(4) for representative locations in the Kissimmee basin are also necessary along with the assumed number of cascades in layer i (CNR (i).

ROUTING MODEL

Purposes:

In our specific investigations, the basic purposes of developing routing methodology are: (1) to distribute sub-basin model output through the system of the lakes, channels and controlling structures, (2) to combine stage-storage fluctuations of the lake with the stage-discharge characteristics of the channel sections for developing a simple joint methodology of reservoir and channel routing, (3) to include operational characteristics of the controlling gates coupled with the routed simulated stages for estimating discharges through various controlling structures, (4) to improve sub-basin model output by including the key process (if any) of the lake or channel which might be excluded from the assumed conceptual physical system, and (5) to provide the basis for examining the effects of changing operational parameters on the hydrologic characteristics of the Kissimmee water system with complete independence from the analysis of the historical data.

Input Information and Essential Formulations:

Input information: While trying to demonstrate the routing model for a one year period of 1970, it is essential to obtain hydrologic base line information just before this period for all the lakes, channels, and controlling structures. Such information (also known as initial conditions) includes: (1) the recorded stages at 14 lakes of the upper and lower Kissimmee, (2) recorded tailwater and headwater elevations at 14 controlling structures, (3) proportioning factors for distributing sub-basin model output in corresponding lakes of a particular planning unit, (4)various constants to convert monthly pan evaporations to 3 hour lake evaporation values.

Essential Formulations:

As an essential part of the simulation procedure, our methodology also depends heavily on the formulations of various water systems. Basic forms of the equations which are used in our analysis are summarized in Table 1. As shown in this table, formulations are classified according to the type of system (i.e., lake, channel or controlling structures). They are described below.

Formulations for lake system: Essentially, the parameters which are useful in the simulation are stages, storages, inflows and outflows for various lakes. The first two equations of the lake system given in Table 1 tie together, change in storage (ΔS) and changes in stage to the characteristics of inflow, outflow and initial stages. These equations are simple forms of mass-balance equations. In addition, it is also necessary to know the stage-storage relationships for all the lakes of the upper Kissimmee. These relationships can be in either tabular form or in mathematical form.

Formulations for controlling structures: Operational characteristics of the Kissimmee water systems are reflected in the formulations of the controlling structures. Variables considered in these formulations are gate openings (GO), headwater elevation (HWE), and tailwater elevation (TWE) with discharge as a dependent variable as shown by Equation 1 for structure operations in Table 1. In the routing methodology these equations are used to compute the discharge through the structure knowing the simulated tailwater and headwater stages for a given set of gate openings.

Channel formulations: The development of the channel formulations and using them in a convenient fashion in routing methodology are some of the steps that make our procedure different than previously attempted techniques. Essentially, the hydraulic formulations given in Table 1 for the channel system relate to: (1) a differential equation representing gradual varied flow with slope of energy line, channel bottom slope, discharges, cross-sectional area, top width of the channel and velocity head coefficients as variables and rate of change of depth (with distance) as a dependent variable (Equation 1 of Table 3), (2) Manning's equation combining hydraulic characteristics of the flow (i.e., velocity, Manning's coefficients, slope of energy line) with the physical characteristics of the channel cross-sections such as cross-sectional area (A) and perimeter (P). (Equation 2 of Table 1 of channel system.), (3) an interative equation based on a numerical integration technique of trapezoidal rule applied by Prasad[6] to estimate the water depth (and then water surface elevation) at the end of the channel section (Equation 3 of Table 1 of the channel system). Using these formulations, the existing FCD backwater program is run to perform backwater computations for all the 25 channel sections of the Kissimmee with the available channel cross-sectional data. For a given channel section, the program generates a set of upstream, downstream stages along with discharges and storages. Using this data set, empirical relationships based on statistical principles are derived for these variables. These established mathematical relationships (also known as backwater functions) are then used in the program to replace directly the backwater computational steps. Among many developed equations, the selected formulations are given in Tables 2, 3, and 4. For better accuracy, these formulations are used in conjunction with corresponding correction factors. The rationale and different points for developing these equations are discussed in detail by Shahane, et al.[7]

COMPUTATIONAL METHODOLOGY

After developing various pieces presented earlier, the next important step is to link them together to distribute the sub-basin flows through the lake, channel, and controlling structures of the Kissimmee basin. Among other possible procedures, the selected method is described briefly in the following section.

At the outset, the three lakes system is considered with emphasis on the middle lake and the associated two channel sections (i.e., one on each side of the middle lake). Using the recorded initial stage of the middle lake, its initial storage is computed from a stage-storage values. From the initial recorded stages of the three lakes, the initial discharges are estimated by channel formulations given in Table 5. If a controlling structure is located in one or both channel sections, the initial discharges are computed from the discharge rating curves for controlling structures knowing the recorded tailwater, headwater elevations (TWE and HWE) and the 3 hour gate opening data. Using these initial estimates of discharges flowing into or away from the middle lake and the local inflow generated by the subbasin model, the change in storage (ΔS) in the middle lake is estimated from the simple mass-balance equation. Knowing the initial storage and the computed change in storage, a new storage and new stage is obtained for a prescribed time step. If the new discharges corresponding to the new stage make the change in storage (ΔS) in the middle lake significantly different than the previously estimated S, then S is again computed using the average values of the new and previous discharges through two channel sections. This iterative procedure is continued until the difference between previous and new estimates of ΔS is within the prescribed limit. At the end of the iteration, final estimates of discharges through the channels, and the lake stage of the middle lake are obtained. These steps are repeated for the next three lake systems and continued for each lake system starting from Alligator Lake to Kissimmee Lake and for five channel systems of the lower Kissimmee basin using all the formulations shown in Tables 2, 3, and 4. Other details of the computational methodology are discussed by Shahane, et al.[7]

RESULTS AND VERIFICATIONS

Results:

After putting together the pieces of the water quantity model as shown in Figure 9, the output is essentially the net result of the interactions of various sub-components of such hydraulic simulation procedure. The primary output from such methodology consists of (1) simulated hydrologic parameters such as sub-surface flow, total losses, deep seepage, available storage in the soil, storage in depression and mean streamflows for 19 planning units on a 3 hour basis, (2) 3 hours simulated discharges through all the channel sections of the upper and lower Kissimmee for the year 1970, (3) 3 hours simulated mean discharges through all the control structures for the full year of 1970, (4) 3 hours simulated stages for 14 lakes of the upper Kissimmee basin, (5) 3 hours simulated tailwater and headwater stages at all the control structures of the upper and lower Kissimmee basins, (6) storages in all the major lakes and storages for five sections of the lower Kissimmee at the end of every 3 hours for the entire year of 1970.

Verifications:

The methodology of the sub-basin model was first applied by previous investigators to the Taylor Creek drainage basin of 100 square miles located on the north side of Lake Okeechobee in Florida. Since the hydraulic, hydrologic and agricultural characteristics of the Taylor Creek watershed are well monitored by the ARS of the U. S. Department of Agriculture, and since this drainage area was in its natural form with no control structures to change its natural drainage characteristics during the test period, it was an ideal place to verify and test the FCD sub-basin model. The typical result of such an effort is depicted in Figure 5 which indicates clearly the adequacy of the sub-basin model and suggests the appropriate choice of coefficients covering the key hydrologic processes.[8,9]

When the same sub-basin model is applied to the 19 drainage basins (also known as planning units) of the Kissimmee, the streamflows at the mouth of these drainage areas are generated. These values are compared with the available yearly historical data (with wet and dry period values) compiled by the Hydrology Division of the FCD. The typical graphical comparison is shown in Figure 6. Based on this comparison, it appears that the sub-basin model simulates hydrologic components which are in general agreement with the recorded values.

The success of the routing methodology can be viewed in terms of the various comparisons of simulated stages and discharges with the corresponding recorded values. The results of our routing methodology for the upper Kissimmee basin were compared with the historical values using a particular set of state conditions, basin parameters of sub-basin models coupled with a specific set of proportioning factors, tabular values and mathematical formulations of the routing model. A typical comparison is shown in Figure 7. Although the correlations depicted in Figure 7 for discharges are excellent, the comparative graphs of simulated and recorded stages of some of the lakes of the upper Kissimmeeshow significant differences. To illustrate this point, typical results in the form of graphical comparison for Lake Tohopekaliga are depicted in Figure 8. These comparisons indicate clearly, (1) the capability of our overall framework of operational watershed model to comvine the sub-basin model with the routing methodology and to generate the wanted simulated information, (2) the relative importance of gate openings as against the head difference across the structure in the discharge rating formulations for the control structures, and (3) the adequacy of the developed operational water quantity model for considering the interactions of stage-storage and discharge characteristics of lakes, canals and controlling structures, making it possible to further examine the effects of changed conditions on the different parameters under investigation.

CONCLUSIONS

1. After designing, formulating, modifying and refining various component parts of the operational water quantity model as shown in Figure 3, it is demonstrated that the hydrologic and hydraulic performance of the controlled water system for a given set of rainfall distribution and gate operations can be adequately simulated.
2. With a realistic framework of assumptions, simplifications and approximations the developed computer program (which takes about 5 hours of computer time for one year of simulation on the CDC 3100 computer) is shown to be successful in performing the following operations: (a) simulating hydrologic parameters (such as sub-surface flow, surface flow, evaporation losses, deep seepage loss, available soil storage, storage in depression and finally streamflows) on a 3 hour basis for 19 planning units using rainfall, state conditions and basin parameters as input data for the year of 1970, (b) routing these generated streamflows of 19 planning units through the controlled system of lakes, channels and operating structures, (c) simulating 3 hour lake stages, headwater and tailwater elevations at structures and discharges through the structures of the upper and lower Kissimmee, (d) comparing the simulated values with recorded values in terms of plotted graphs and tables, and (e) performing parametric sensitivity analysis by changing the key parameters of the

sub-basin model and the routing model.

3. It appears that the developed model can be directly or indirectly useful in (a) examining the effects of certain physical parameters on the final outcome of discharges and stages, (b) providing operational information regarding the required set of gate openings to maintain water levels and discharges at a particular level at specific locations, and (c) utilizing the generated hydrologic information in the other practical aspects of water management.

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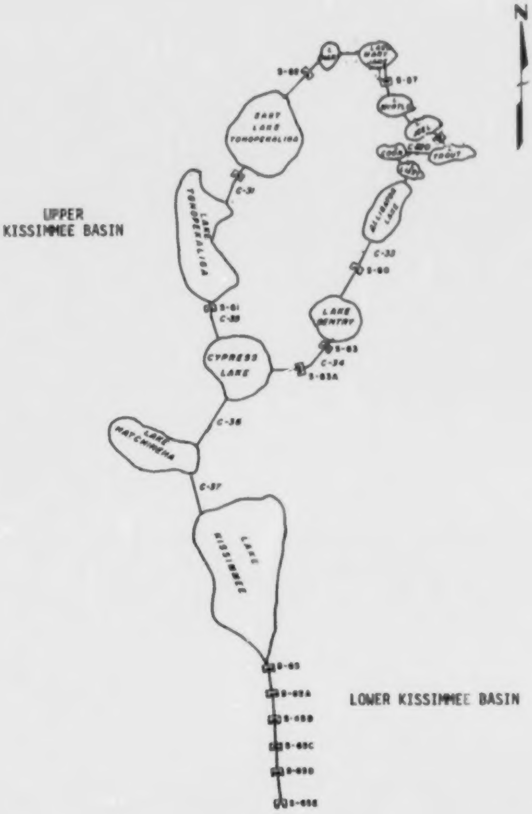
NOTATIONS

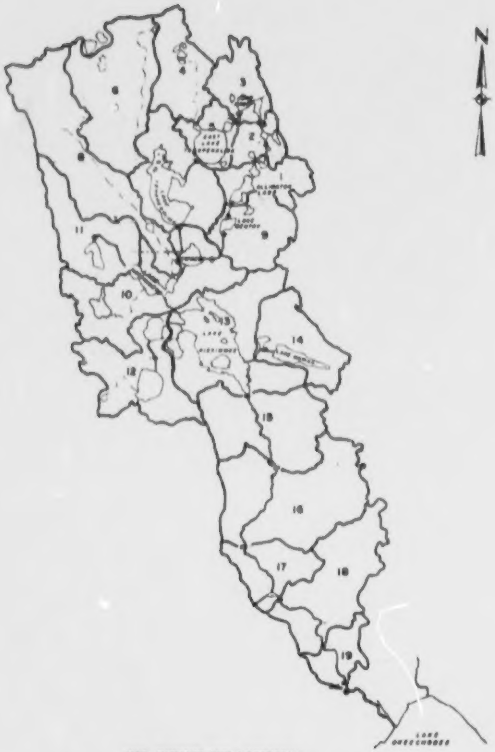
ΔS	change in storage,
WSE	water surface elevation,
S	storage,
SO	bottom bed slope,
SE	slope of the energy line,
n	Manning's coefficient,
V	velocity,
HR	hydraulic radius,
Q	discharge,
A	cross sectional area,
Y	depth,
GO	gate opening,
EH	headwater elevation (HWE) - tailwater elevation (TWE),
DX	distance between reaches i+1 and i,
α	velocity head coefficient,
T	top width of the channel,
g	gravitational acceleration,
a,b,p,r,s	constants



SCHEMATIC REPRESENTATION OF THE
CHAIN OF UPPER KISSIMMEE LAKES AND LOWER KISSIMMEE FIVE POOLS

NOT TO SCALE

FIGURE 1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LAKE OKEECHOBEE

MAP SHOWING THE LOCATIONS
OF THE 19 PLANNING UNITS OF THE KISSIMMEE BASIN

Figure 2

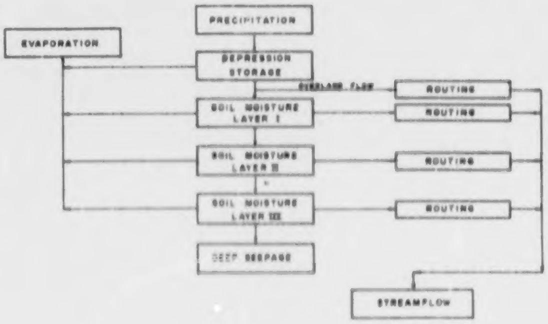

PRECIPITATION
EVAPORATION
DEPRESSION STORAGE
OVERLAND FLOW
ROUTING
SOIL MOISTURE LAYER I
ROUTING
SOIL MOISTURE LAYER II
ROUTING
SOIL MOISTURE LAYER III
ROUTING
DEEP SEEPAGE
STREAMFLOW

Figure 4 F.C.D. SUB-BASIN MODEL

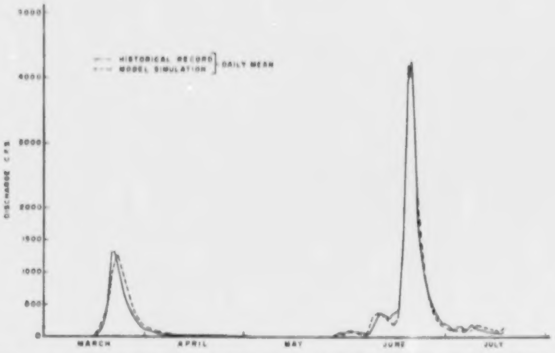


Figure 5 COMPARISON OF SIMULATED AND RECORDED DISCHARGE FOR TAYLOR CREEK (8,9)

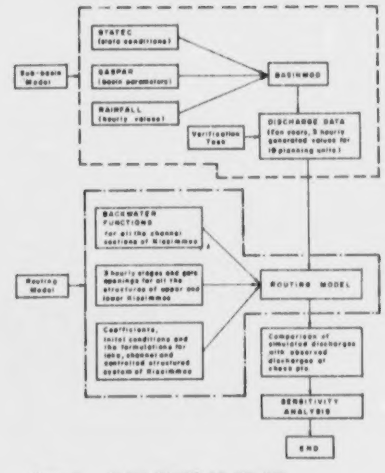
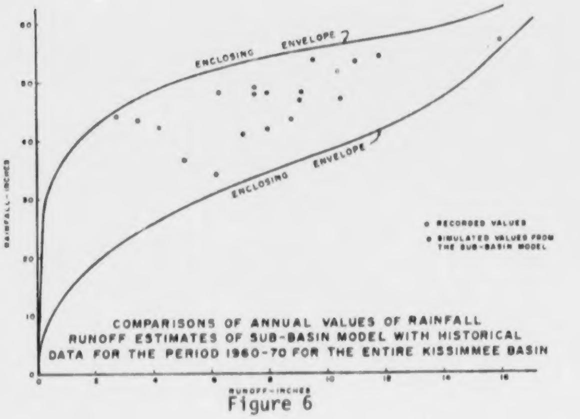
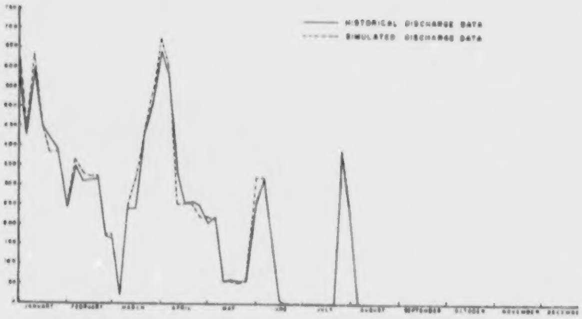

Sub-basin Model
STATEC (state conditions)
GASPAR (basin parameters)
RAINFALL (hourly values)
BASINMOD
Verification Test
DISCHARGE DATA (Ten years, 3 hourly generated values for 19 planning units)
Routing Model
BACKWATER FUNCTIONS for all the channel sections of Kissimmee
3 hourly stages and gate openings for all the structures of upper and lower Kissimmee
Coefficients, initial conditions and the formulations for lake, channel and controlled structured system of Kissimmee
ROUTING MODEL
Comparison of simulated discharges with observed discharges at check pts.
SENSITIVITY ANALYSIS
END

Figure 3 FLOW CHART OF MAJOR COMPUTATIONAL STEPS INVOLVED IN F.C.D. WATER QUANTITY MODEL



COMPARISONS OF ANNUAL VALUES OF RAINFALL RUNOFF ESTIMATES OF SUB-BASIN MODEL WITH HISTORICAL DATA FOR THE PERIOD 1960-70 FOR THE ENTIRE KISSIMMEE BASIN

Figure 6



COMPARISON OF SIMULATED AND RECORDED DISCHARGES THROUGH S-59 FOR THE FULL YEAR OF 1970

Figure 7

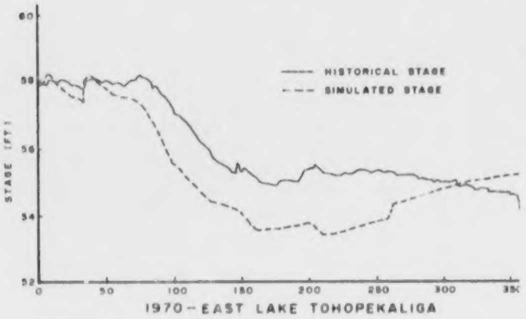


Figure 8 COMPARISON OF SIMULATED AND RECORDED STAGES FOR EAST LAKE TOHOPEKALIGA FOR THE YEAR 1970

Table 1. Basic forms of equations useful in the model.*

System		Formulations	
Lake System	1.	$(\text{stage})_{t+1} = (\text{stage})_t +$ [illegible] $_{t+1}$	(A)
	2.	$(\Delta S)_{t+1} = I_{t+1} - O_{t+1}$	(B)
	3.	$WSE = a\,(S)^b$	(C)
	4.	polynomial equations	
		$\text{stage} = A_0 + A_1(S) + A_2(S)^2 + A_3(S)^3 + A_4(S)^4$	(D)
Channel System	1.	$\frac{dy}{dx} = \frac{SO - SE}{1 - \frac{aQ^2T}{gA^3}} = \psi$	(E)
	2.	$SE = \frac{(n)^2V^2}{2.22\ (H.R)^{4/3}}$	(F)
		$SE = \frac{n^2Q^2P^{4/3}}{2.2\ A^{10/3}}$	
	3.	$Y_{i+1} = Y_i + [\frac{\psi_{i+1} + \psi_i}{2}]\ DX$	(G)
Structures Operations	1.	$Q(H) = P(GO)^r\ (EH)^S$	(H)

*Notations are explained at the end of the paper.

Table 2. Nonlinear formulations of discharges for the typical seven channel sections of the upper Kissimmee basin.

Channel Section	Nonlinear Relationship $Q = (US-DS)^A\ (DS)^B$		
	A	B	r^2
C-32G	0.19562817	1.37327452	0.99036109
C-32B	0.12933563	1.31192007	0.99028838
C-32D	0.11312801	1.28232715	0.98835559
C-32F	0.02812316	1.14778715	0.98488793
C-29	0.23189354	1.53817995	0.99206125
C-37	0.44362025	2.25302023	0.99901088
C-36	0.40565648	2.17679705	0.99862609

r = correlation coefficient,

Q = mean discharge,

US = upstream stage,

DS = downstream stage

Table 3. Stage-storage-discharge relationships for the lower Kissimmee basin.

Channel Section *	Nonlinear Relationship $US = (DS)^A(\log Q)^B$		
	A	B	r^2
C-38A	0.93525909	0.12357836	0.99999427
C-38B	0.80300638	0.34915258	0.99997801
C-38C	0.72539726	0.45337676	0.99993335
C-38D	0.72979747	0.42254163	0.99995117
C-38E	0.84436366	0.22342889	0.99995183

r = correlation coefficient,

US = upstream stage,

DS = downstream stage,

Q = mean discharge,

$Q > 0$

* C-38A = channel section of C-38 between structures S-65 and S-65A
C-38B = " " " " " " S-F5A and S-65B
C-38C = " " " " " " S-65B and S-65C
C-38D = " " " " " " S-65C and S-65D
C-38E = " " " " " " S-65D and S-65E

Table 4. Stage-storage-discharge relationships for the lower Kissimme basin.

Channel Section	Nonlinear Relationship $DS = (\log Q)^A(\log ST)^B$		
	A	B	r^2
C-38A	0.46661167	1.29225620	0.9974083
C-38B	0.06123664	1.59817418	0.99994493
C-38C	-0.11387716	1.70097296	0.99985066
C-38D	-0.32464046	1.79672855	0.99987939
C-38E	-0.31844141	1.68094907	0.99921370

r = correlation coefficient,

DS = downstream stage,

Q = discharge,

ST = storage in acre ft.,

$Q > 0$

HOW TO MAKE SIMULATIONS MORE EFFECTIVE

George S. Fishman
University of North Carolina
Chapel Hill

Discrete event simulation on a digital computer has been with us as a tool of analysis for over two decades. Among the attractions it offers are the ability to model detail (where analytical methods fear to tread) and the ability to control variation (which real world experimentation cannot). The first of these abilities, modeling detail, seems to have been oversold, and the second, control of variation, has been undersold. The presentation concentrates on these two topics, offering examples and guidance as to how thoughtful reflection on these two areas, before simulation modeling and programming begin, can lead to more effective use of the simulation method.

1. Introduction

In today's presentation my remarks are intended to put the problems that arise in a simulation on a digital computer in perspective and to offer direction in solving some of the statistical ones. Hopefully, this perspective and direction will facilitate our discussion here on just what can be done to increase user satisfaction with the building blocks of simulation.

2. Features of the Simulation Method

As a tool for studying complex systems, simulation offers many attractions. These include:

1. compression of time
2. expansion of time
3. model detail
4. selection of outputs
5. control of measurement errors
6. control of variation.

A properly constructed simulation model can compress time so that several years of system activity can be simulated in minutes or, in some cases, seconds. This ability enables one to run through a variety of operational designs of interest in a fraction of the time required to try each on the real system.

The ability to expand time also has its benefits. By arranging for statistics of interest to be produced over small intervals of simulated time, one can study the detailed structure of system change that cannot be observed in real time. This figurative time dilation is especially helpful when little data exist on change in the real system.

Model detail is often cited as the most notable feature of computer simulation. Although all modeling involves some abstraction from reality, the ostensible reason for using simulation in the minds of many analysts is that it allows them to model detail that other methods would have to omit in order to admit a solution. This ability to include detail has occasionally led to a euphoria about what simulation can do. Unfortunately the dark side of the picture is seldom mentioned in advance and inevitably a user who exploits this ability to include detail learns that all is not well at a later stage in his use of simulation. Section 3 discusses the subject of detail with regard to its dark side in depth.

The ability to select output and reports of varying degrees of detail also contribute to the appeal of simulation. However, it should be remembered that the computation of output statistics take time. Therefore, a judicious simulation user devotes prior thought to what the relative importance of different outputs is and to the ways in which he can manipulate a small internal data base to produce many outputs of interest. For example, in a queueing system the identity $L = \lambda W$ where L denotes mean queue length; λ, the arrival rate; and W, the mean waiting time holds under fairly general conditions. Therefore, one need collect data to estimate either L or W since the other can be obtained by either division or multiplication by the known arrival rate λ.

Control of measurement errors offers a great comfort to simulation users. Presumably the automatic fashion in which data are collected in a computer simulation together with the fact that machine errors are virtually absent has, until recently, led to complacency about the possibility of error. With the advent of the simulation of computer systems in which the time between events is of the order of microseconds but run lengths are of the order of hours, it has become clear that the accumulated simulation time which is generally computed by adding the times between events is subject to substantial error. Whether or not this is a serious issue for a simulation study depends on the nature of interevent times relative to run length times.

Control of variation is the least appreciated feature of computer simulation. This may be a result of the fact that some knowledge of statistics is necessary to exploit this feature. In particular, application of this control of variation enables one to obtain results with a specified accuracy at lower cost than if one ignored the potential for control. Section 4 offers a number of examples to illustrate how easily this exploitation can be made to work.

3. Detail

There exists a general presumption among analysts that if they were just able to make their models conform more closely to the observed behavior, then they would increase chances of having a successful study. Simulation, being a descriptive tool, allows one in theory to make a model as close to resembling reality figuratively as one likes. However, in order to close the gap between model and reality, one has to have a definitive picture of the behavior to be modeled.

To study detail we use a simulation of a fire support system as an example. Fire support involves a host of microphenomena; they include:

- A. target acquisition
  1. detection
  2. identification
  3. location
- B. target engagement
  1. priority rules
  2. weapons availability
  3. weapons selection rules
- C. fire support performance
  1. target characteristics
  2. weapons characteristics
  3. measures of effectiveness.

Each calls for detail which hopefully would arise from actual battlefield experience. If the knowledge needed to derive a more adequate representation of target detection, location and identification exists, then one has to decide whether its inclusion in the simulation will improve representational accuracy to an extent that makes the extra modeling effort worthwhile. However, this improvement can only be measured after the fact. In particular, inclusion of known detail in a comprehensive fire support description would have to be preceded by extensive testing of alternative mathematical and logical representations.

To do this one needs *data*.

Every extension of a simulation's detail introduces new parameters. These require estimation which relies on data, whether it be sample observations or expert judgment. Naturally the more detail that is desired, the more data that are required. This poses a dilemma for the analyst. While he may be able to describe a phenomenon conceptually, he may not have the data needed to fit the parameters of the corresponding mathematical representation. If he does have the data, he must then face the issue as to how representative the parameter estimates are when this particular micromodel is used in a variety of alternative settings. That is, parameter values may be a function of the setting in which the model is used and, therefore, an analyst may need several sets of data to estimate the values that parameters assume in different settings.

The third dark issue that more detail induces is increased bookkeeping and computation in a simulation computer program. More detail implies more events or state changes per unit time in the model. From a programming viewpoint this requires additional data structures and logical structures. This requirement adds to the cost of putting the program together. Although it is true that languages such as GPSS and SIMSCRIPT II make these supplements relatively easy to introduce representationally, an analyst is still faced with the problem of *fitting* his program into the computer on which he plans to do his work.

If FORTRAN is used for modeling then a serious additional problem arises. Fire support simulation involves relatively intricate time sequencing of many diverse events. Whereas specialized simulation programming languages all contain *timing routines* that perform this time sequencing automatically, the user of FORTRAN must build his own timing routine. This effort alone can be so cost consuming as to defeat the purpose of using FORTRAN for its computational efficiency. In particular, FORTRAN lacks a list processing capability, a principal feature of all simulation programming languages. For this reason alone one has to question the flexibility and versatility of a fire support model programmed in a language other than a simulation programming language.

The effect of detail on program development represents only one issue in this area. Detail seriously affects program execution also. In addition to creating more data and logical structures, more detail causes more events to occur per unit time in a simulation. This implies that the list of scheduled events on which the timing routine relies for direction is longer. This means that when a new event is to be scheduled the timing routine takes more CPU time to find the correct position for the corresponding event notice in the list of schedule of events.

Unfortunately the current state of development of most simulation languages have contributed to the seriousness of this problem in practice. In order to retain a simplicity in list structures and processing for general simulation, these languages search, add and delete from these lists using algorithms that in no way exploit the nature of the event list for particular problem settings. Moreover, many simulation users do not recognize that alternative ways exist to process the list of scheduled events as well as other lists that materialize during the course of a simulation.

By now, many people recognize that the generality of simulation programming languages may represent an impediment to computational efficiency in the fire support area. This recognition has led to a proposal there for more tailoring to the needs of this kind of simulation. This idea deserves encouragement. However, one hopes the tailoring will not be restrictive of the resulting simulation programs' use for alternative fire support studies. Using a simulation language to formalize concepts and structures would help to insure this generality.

Few, if any, tailored simulations have been reported in the literature. What has been reported are ways to speed up list processing in general. One suggestion which most experienced simulation users follow, regardless of the problem, is to create a single event notice for two diverse events that always occur simultaneously. Then a subroutine call within the executable code of one of the events enables the other event to be executed. A second suggestion concerns conditionality. Occasionally one event occurs only after another type of event has occurred. However, the second event does not always occur. In this case an event notice for the necessary event is generated in the simulation and within the executable code for this event a test is made to see if execution of the other type of event has to occur. The effect of these two suggestions is to reduce the number of event notices in the list of scheduled events, thereby reducing the processing time for this list. Unfortunately the very emphasis on events in a language such as SIMSCRIPT encourages a user to overlook the fact that simple suggestions such as these two can considerably shorten execution time.

Recently, other suggestions have appeared in the literature. The papers by Vaucher and Duval [9] and Wyman [10] in the *Communications of the ACM* relate experience with alternative search procedures aimed at reducing list search time. In GPSS the judicious user of a *user chain* to shorten the length of the *current events chain* offers dramatic savings, when properly used [6].

Improved processing of other lists can also induce efficiencies in large scale simulation. For example, suppose that available resources in a fire support simulation are all kept on a single *available resource* list. Presumably the type of resource is distinguished by a value assigned to its attribute that designates type. Every time a resource is required, a search of the resource list occurs. If there are many available resources of many different types the search is time consuming. Alternatively, if one judiciously constructs several lists based on type then the simulation needs only to search the selected shorter list. The price paid for search efficiency is the increased number of list structures defined in the simulation. The exact balance between the cost of having more lists and the saving in search time depends on the particular system under study.

4. Control of Variation

Although control of variation seldom receives serious attention in large scale simulation, it is in this writer's mind one of the most attractive features of the simulation method. Control of variation includes the ability to control the pattern of variation in the streams of random numbers that serve as input to an ongoing simulation. Thoughtful use of this ability enables a user to attain a desired statistical accuracy with less computer time than neglect of the option would require. This benefit can accrue when running replications of an experiment in which all input parameters are the same. It can also occur when comparing runs of an experiment in which at least one of the input parameters assumes different values. An example illustrates the point.

Consider an airline reservation office with m reservationists. If at least one reservationist is idle when a call occurs the call immediately receives service. If all reservationists are busy the caller listens to a 9 second recorded message excusing the delay. At the end of the message the caller receives service, if a reservationist is available. Otherwise, he is put into a queue with first-come-first-served discipline. Intercall times follow an exponential distribution with mean $1/\lambda$. Each caller makes a one-way reservation with probability 1-p and a round trip reservation with probability p. Service times for one way trips are exponential with mean $1/\omega$. Round trip service times are Erlang with shape parameter 2 and mean $2/\omega$. Times are in minutes.

Consider the case in which $\lambda = 1$, $\omega = 0.5$, $m = 6$, and $p = 0.75$. Suppose one wishes to estimate mean waiting time to within ± 0.025 minutes or, equivalently, ± 1.5 seconds. Let $\bar{Y}_i$ denote sample mean waiting time on replication i. Let

$$(1) \quad \bar{Y}_k = k^{-1} \sum_{i=1}^{k} Y_i \qquad s^2_k(Y) = (k-1)^{-1} \sum_{i=1}^{k} (Y_i - \bar{Y}_k)^2.$$

Suppose we adopt the following design for our experiment: Continue to collect independent replications until [1]

$$s^2_k(Y) \leq k(0.025)^2/t^2_{k-1}$$

where t_{k-1} is the .975 significance point of the t distribution with k-1 degrees of freedom. Then if $Y_1, \ldots, Y_k$ are normally distributed the probability that $\bar{Y}_k$ is within ± 0.025 of the true waiting time is approximately† 0.95. Table 1 shows the results using independent replications.

This particular simulation was run in SIMSCRIPT II.5 with intercall times generated on stream 1, service times on stream 2 and type of call (one way or two way) on stream 3. In a simulation of a single server queueing system Page [7] has shown that reversing the streams of random numbers for interarrival and service times on a second replication can induce sizable variance reductions. Presumably, low interarrival times and high service times produce high congestion on the first run whereas reversal of streams produces high interarrival times and low service times and. therefore, low activity on a second run. Therefore, average sample output over the two runs should have a smaller variance than in the case of independent replications.

Table 2 presents the results of reversing seeds on streams 1 and 2 on pairs of replications. In order to allow comparison with Table 1, the experiment here was designed to have about half as many completions per run as in Table 1. The results in Table 2 indicate that only 12354 completions were required to obtain the same statistical accuracy as in Table 1, which required 25543. In terms of variance one has

$$(2) \quad s^2_5(X) = 7.55 \times 10^{-4} \qquad s^2_5(Z) = 23.34 \times 10^{-4}.$$

Then one way to measure variance reduction is to examine the simple ratio

$$(3) \qquad [s^2_5(X) + s^2_5(Z)]/4s^2_5(Y) = 2.03$$

which indicates that seed switching has cut the variance by about one half.

Other methods of controlling variation are also available. Let X and Y have means μ_x and μ_y, respectively. Suppose that μ_x is known but μ_y is to be estimated. One estimate is Y, another is $Z = Y + c(X - \mu_x)$ for which $\mathrm{var}(Z) \leq \mathrm{var}(Y)$ if

$$(4) \qquad c \leq -2\,\mathrm{cov}(X,Y)/\mathrm{var}(X).$$

Consider the airline reservation problem again and let X denote the sample intercall time, $\mu_x = 1/\lambda$ and $c = 1$. The choice of c is based on the observation that if $X - \mu_x$ is positive the intercall times in a replication are above average and, therefore, congestion and waiting time are below average.

Table 3 presents the results of using intercall time as a control variate. The extent of variance is evident.

When comparing results on experiments with different inputs, variance reduction is again possible. These range from using common seeds for corresponding streams to varying the number of observations collected on each run [3]. For example, suppose that one wants to measure the reduction in mean waiting time that accrues when the number of reservationists increases from 6 to 7. Moreover, the accuracy required is d = 1/60 minutes or 1 second.

Table 4 shows the results when common seeds are used for corresponding streams on corresponding runs. Since

$$(5) \quad s^2_3(X) = 4.4 \times 10^{-4} \qquad s^2_3(Z) = 2.10 \times 10^{-4}$$

variance reduction is estimated to be

$$(6) \qquad [s^2_3(X) + s^2_3(Z)]/s^2_3(Y) = 15.5,$$

impressive by most standards.

In some simulation settings it is not possible to match seeds or to induce the necessary correlation between runs to effect a variance reduction. This is especially true when comparing the results or radically different experiments. Here one may have to settle for independent replications, however, variance reduction can still occur. Consider two experiments with outputs X and Z and sample sizes per replication of n_x and n_z. Let $\mathrm{var}(X) = \sigma^2_x/n_x$ and $\mathrm{var}(Z) = \sigma^2_z/n_z$ under the assumption that one is able to create independent observations within each replication[(2, 4]. Let c_x and c_z denote the unit costs of collecting and processing observations in each replication. If one wants to achieve a specified variance $V = \sigma^2_x/n_x + \sigma^2_z/n_z$ for $Y = X - Z$ on each replication then n_x and n_z should be selected so that

$$(7) \qquad \begin{array}{c} r = n_x/n_z = r_1/r_2 \\ r^2_1 = \sigma^2_x/\sigma^2_z \qquad r^2_2 = c_x/c_z . \end{array}$$

Using (7) with $n_x + n_z = n$ instead of $n_x = n/2$ leads to a saving in computing cost of $(r_1 - r_2)^2/(1 + r^2_1)(1 + r^2_2) \times 100$ percent.

In preliminary runs of the simulation for $m = 6$ and 7 we estimated $\hat{\sigma}^2_x/\hat{\sigma}^2_z = 5.5$ and $\hat{c}_x/\hat{c}_z = 0.95$ so that $r = 2.41$. Ten replications of each experiment were run with $n_x = 600$ and $n_z = 250$. Upon computation of the appropriate terms the estimated saving in computer time needed to achieve the resulting variance for $\bar{Y}_k = \bar{X}_k - \bar{Z}_k$ was about one third. From this one has to deduct the cost of the two preliminary runs; but that cost was incidental.

The methods of variance reduction discussed here represent a few among many techniques. All exploit the structure of the individual problems to a marginal extent only. However, methods do exist that exploit the properties of individual problems in such a way that substantial variance reductions are possible. These are discussed in [3, Sections 11.2 - 11.3].

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† See [8] for details.

5. References

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Table 1

Sequential Estimation of Mean Waiting Time

d = 0.025 minutes, significance level = 0.05

k	Y_k	$\bar{Y}_k$	$s^2_k(Y)$ (10^{-4})	kd^2/t^2_{k-1} (10^{-4})	No. of Completions
1	0.2243	0.2243			2651
2	.1705	.1974	14.47	0.08	2497
3	.1721	.1890	9.37	1.01	2781
4	.1619	.1822	8.08	2.47	2500
5	.1583	.1774	7.20	4.06	2629
6	.2275	.1858	9.94	5.67	2550
7	.2222	.1910	10.18	7.31	2595
8	.1576	.1868	10.12	8.94	2422
9	.2362	.1923	11.56	10.58	2440
→ 10	.2138	.1944	10.74	12.22	2478
					25543

Table 2

Sequential Estimation of Mean Waiting Time

Using Seed Switching

d = 0.025 minutes, significance level = 0.05

k	X_k	Z_k	$Y_k = (X_k+Z_k)/2$	$\bar{Y}_k$	$s^2_k(Y)$ (10^{-4})	kd^2/t^2_{k-1} (10^{-4})	No. of Completions
1	0.1649	.1699	0.1674	0.1674			1262 + 1335
2	.2240	.2338	.1739	.1707	2.11	0.08	1255 + 1113
3	.2250	.1679	.1965	.1893	2.33	1.01	1165 + 1220
4	.1755	.2483	.2119	.1874	4.22	2.47	1352 + 1251
→ 5	.2618	.1373	.1695	.1838	3.81	4.06	1178 + 1223
							12354

Table 3

Sequential Estimation of Mean Waiting Time

Using a Control Variate

d = 0.025, significance level = 0.05

k	Z_k	$\bar{Z}_k$	$s^2_k(Z)$ (10^{-4})	kd^2/t^2_{k-1} (10^{-4})	No. of Completions
1	0.2100	0.2100			2651
2	.1648	.1874	10.22	0.08	2497
3	.1760	.1836	5.54	1.01	2781
4	.1528	.1759	6.07	2.47	2500
5	.1624	.1732	4.91	4.06	2629
6	.2079	.1790	5.94	5.64	2550
→ 7	.2134	.1839	6.64	7.31	2595
					18203

Table 4

Sequential Estimation of Mean Waiting Time Difference

d = 1/60 minutes, significance level = 0.05

k	X_k m=6	Z_k m=7	$Y_k = X_k - Z_k$	$\bar{Y}_k$	$s^2_k(Y)$ 10^{-4}	kd^2/t^2_k-1 10^{-4}
1	0.1884	0.0628	0.1256	0.1256		
2	.1575	.0411	.1164	.1210	0.42	0.03
→ 3	.1976	.0687	.1289	.1236	0.42	.45

THE FACTUAL BACKGROUND OF ECOLOGICAL MODELS:
TAPPING SOME UNUSED RESOURCES

E. C. Pielou

Biology Department, Dalhousie University,
Halifax, Nova Scotia, Canada

Summary

Successful ecosystem modeling on a large scale requires knowledge of the relative performance of many species in response to changes in numerous environmental variables. Without such knowledge it is impossible to estimate the relative magnitudes, or even the signs, of the numerical constants in prediction equations. Acquiring this knowledge is difficult, expensive, and time-consuming. If the information now stored in the ecological literature and data banks can contribute, it should be used.

Much information exists on biogeographic and ecological zonation patterns, and it constitutes a particularly rich source for deriving new ecological insights from old data. This paper describes two new ways of analyzing such data. One entails determining the overlap score of a group of species in order to judge whether the species are competing. The other (incompletely developed) method entails comparing coefficients of concordance in order to judge the relative importance of different environmental factors in controlling community composition.

Introduction

Most theoretical ecologists, and hence the applied ecologists who consult them, are aware of a growing split in their subject. It has two separate, diverging areas. One is "mathematical" ecology and the other "statistical" ecology. However, ecology per se is still one subject and the unfortunate divergence of its parts is merely because of the styles of mathematical argument employed and the kinds of theoreticians who practice them.

For the most part, theoretical modeling in ecology has been the work of mathematical, as opposed to statistical, ecologists. Models of many kinds all have two indispensable ingredients, or sets of ingredients: processes and parameters. The processes are the changes in size and age structure of interacting living populations, and the accompanying flows of energy and materials, as modeled by equations. Whether these are simple linear regression equations or esoteric non-linear integro-differential equations, they are still "forms" with (temporarily, at least) no numerical content. The parameters are the numerical coefficients (or, for studies of qualitative system stability, the signs of the coefficients) that must be entered in the process equations before any concrete predictions can emerge.

Now consider from where the numbers are to come. There are various possibilities. Educated guesses are one source, to see how the model (i.e., the process) will behave in a wide range of conditions.

A second source is experiment. For example, if processes in such microcosms as Paramecium species in vials of water or Tribolium species in vials of flour are to be modeled, the birth and death rates and the growth and feeding rates of the animals, and the way these rates vary in response to changing abiotic conditions can, with persistence and patience, be discovered by experiment.

A third source of numerical parameters is observation of the system to be modeled, itself. This is the customary procedure when a "statistical model" - a hypothesized statistical distribution - is to be fitted to an empirical frequency distribution. The data are first made to yield the desired parameters, with the familiar loss of degrees of freedom and, of course, generality.

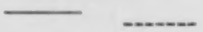
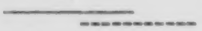
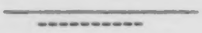
A fourth source of numbers is the vast accumulation of miscellaneous ecological data, reposing in the literature and in various data banks, gathered for purposes of every conceivable kind. A body of data gathered for one purpose is available, if it has been suitably stored, for another purpose; not to use hard-won data in as many ways as possible is wasteful in the extreme. Admittedly, to expect data collected for one purpose to yield the precise coefficients required for an unrelated ecological model to be "run" is probably to expect too much. However, some kinds of data can certainly yield useful information. For example, the data on the zonation patterns of plant and animal species, both "regional" (along short environmental gradients a few kilometers long) and "geographical" (along long gradients, typically latitudinal gradients, of perhaps thousands of kilometers) could yield useful information.

Much published data exist on regional (or ecological) and geographical (or biogeographical) zonation. They obviously tell something about the tolerance ranges of different species in response to different abiotic environmental factors, and about the relative importance of the various factors. They also tell something about the way species interact, and the ways in which their interactions vary from place to place. Thus, perhaps, one can learn whether groups of related species do in fact compete, instead of postulating they compete and inferring a result that is merely conditional on the correctness of the postulate. It is obviously worthwhile to devise ways of ransacking existing data on zonation for useful information that can be fed into, or at any rate can inspire, models. This paper describes two rather tentative approaches to the task.

Competing Species and Overlapping Zones

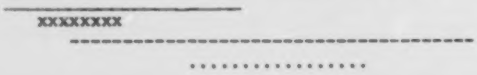
Everyone knows that related species may occupy somewhat different zones on an environmental gradient. The gradient performs a natural sorting experiment (a laboratory analog is paper chromatography) and each species comes to occupy its characteristic zone. This raises the following question: Do related species, for example, congeneric species, tend to occupy zones whose amount of overlap is slight because of competitive exclusion, either over the short term, or evolving over the long term? Or, alternatively, do their zones tend to coincide because, owing to their common ancestry, their tolerance ranges for the chief factor and its associated factors that vary along the gradient are all fairly similar? To discriminate between these contrasted possibilities, one must set up a null hypothesis: What would be observed if the spatial extents and arrangements of a set of zones were mutually independent?

Consider two species, A and B, of sessile organisms living on a gradient. Suppose their zones are discernible. Label the species' upgradient boundaries A1 and B1 and their downgradient boundaries A2 and B2. Assume that (in the diagram below) the gradient descends from left to right. Then we must have A1 to the left of A2 and B1 to the left of B2 but, under the null hypothesis of zone independence, all permutations of A1, A2, B1, and B2 consistent with these constraints are equiprobable. There are only three such permutations, namely:

In symbols	Graphically	Overlap score
A1 A2 B1 B2		0
A1 B1 A2 B2		1
A1 B1 B2 A2		2

In the graphic representation the zones are assumed to stretch up and down the page and the lines (solid for A, broken for B) show the widths of the zones. Scores to be assigned for the three degrees of overlap are shown on the right.

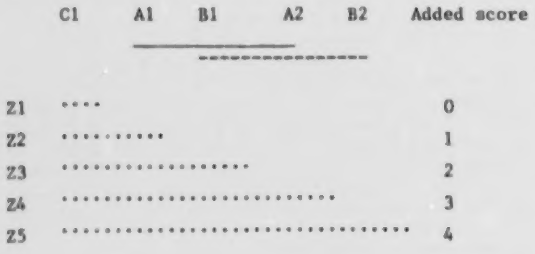
Now suppose there are several, say k, species. We shall assign to their zone pattern a total overlap score, L, which is the sum of the $k(k-1)/2$ pairwise scores reached by taking the species two at a time. For example, for the pattern below in which $k = 4$, the total score is easily found to be $L = 7$.



Observe that the lengths of the lines (representing the widths of the species' zones) are immaterial; it is only the relative arrangement of their boundaries that concerns us.

Now derive the probability distribution, and the mean and variance, of L given the null hypothesis.

Let $f_k(L)$ be the number of ways in which k zones can give a score of L. As shown above, when $k = 2$, $f_k(L) = 1$ for $L = 0,1,2$. Now suppose that to A and B a third species, C, is added. Its upper boundary, C1, is assumed to be to the left of A1 and B1; this assumption does not reduce the number of possible zone arrangements since the species can always be labeled so that their upgradient boundaries are in the order C1, A1, B1. Then, whatever the pattern (and hence the score) of the pair of zones A + B, there are five possible positions for C2 relative to the four existing boundaries A1, A2, B1 and B2. Thus, if the pair A + B has the pattern shown by the solid and broken lines in the diagram below, addition of species C, whose possible zones are the dotted lines, can lead to five distinguishably different patterns labeled Z1,..., Z5. Then, depending on the position of C2 relative to A1, A2, B1 and B2, the total score for all three species together is the sum of the score $L = 1$ that pertains to the A + B pair already, and the "added score" (from C + A and C + B) shown on the right. Moreover, these five equiprobable values for the added score are the same regardless of the score already possessed by the A + B pair.



Hence it will be found that

$f_3(L) = 1$ for $L = 0$ and 6 ;

$f_3(L) = 2$ for $L = 1$ and 5 ;

$f_3(L) = 3$ for $L = 2, 3$ and 4 ;

and $\sum f_3(L) = 15$.

Similar arguments lead straightforwardly to the following recurrence relation for $f_k(L)$:

$$f_k(L) = \sum_{j=L-2k+2}^{L} f_{k-1}(j) \qquad \text{for } L = 0,1,\ldots,k(k-1)$$

with $f_{k-1}(j) = 0$ for $j < 0$ and $j > (k-1)(k-2)$.

The maximum value of L, which is $k(k-1)$, occurs when all $(k-1)1/2$ scores of the zones taken in pairs are equal to 2. From symmetry, it is seen that the mean of L must fall halfway between its extremes.

Therefore $E(L|k) = k(k-1)/2$.

Also put $$\sum_{L=0}^{k(k-1)} f_k(L) = \frac{(2k)!}{2^k\, k!} = T_k \ .$$

Then the probability of obtaining a specified score, L, for given k, is

$$P_k(L) = f_k(L)/T_k \ .$$

The variance of L for given k, namely $Var(L|k)$ is found as follows.

First, put $$V_x(L|k) = \sum_{L=0}^{k(k-1)} (L-x)^2\, P_k(L) \ .$$

That is, $V_x(L|k)$ is the second moment of L about an arbitrary constant x given that the number of species is k. Then, since

$$\sum L P_k(L) = E(L|k) = k(k-1)/2 \ ,$$

$$V_x(L|k) = V_0(L|k) - xk(k-1) + x^2 \ .$$

Now, from the way in which $f_k(L)$ is constructed, it is seen that

$$V_0(L|k+1) = \frac{T_k}{T_{k+1}} \sum_{x=-2k}^{0} V_x(L|k)$$

$$= \frac{1}{2k+1}\left\{(2k+1)V_0(L|k) - k(k-1)\sum_{-2k}^{0} x + \sum_{-2k}^{0} x^2\right\}$$

$$= V_0(L|k) + k^2(k-1) + k(4k+1)/3 \ .$$

Therefore $Var(L|k+1) = Var(L|k) + k(k+1)/3$.

Repeated use of this recurrence relation now shows that

$$Var(L|k) = Var(L|k-1) + (k-1)k/3$$

$$= Var(L|k-2) + (k-2)(k-1)/3 + (k-1)k/3$$

$$\cdots\cdots\cdots\cdots$$

$$= \frac{1}{3}\sum_{1}^{k} (j-1)j \ ;$$

then $Var(L|k) = k(k-1)(k+1)/9$.

The distribution tends to normality with increasing k and for $k \geq 20$ the discrepancy between the true cumulative distribution of L and that of a normal distribution with the same mean and variance nowhere exceeds 1%. For low values of k, the distribution of L is platykurtic. To test the null hypothesis (that the boundaries of the zones of k species occurring on a gradient are independent of one another) when $k < 20$, the critical values C_k tabulated below may be used. These values are for a 5% two-tailed test. That is, if $C_k < L < k(k-1)-C_k$ the null hypothesis should be accepted; (note that C_k itself, and $k(k-1)-C_k$, are included in the acceptance region).

Table 1. Critical Values of L for $k = 2,\ldots, 19$

k	C_k	k	C_k	k	C_k
2	0	8	16	14	62
3	0	9	21	15	73
4	2	10	28	16	85
5	4	11	35	17	98
6	7	12	43	18	111
7	11	13	52	19	126

An example of the use of the test is given in the section, Examples.

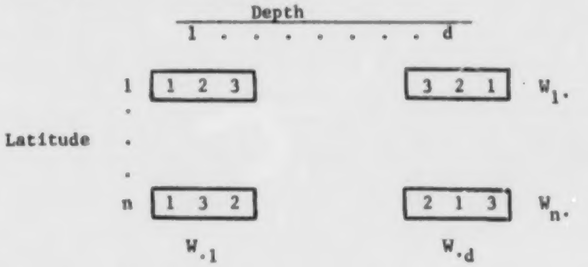
Concordances Among Different Groups of Samples

In this section, an entirely different way is described of extracting, from data on species zonation, information that may be useful to ecosystem modelers. The method is "work in progress" which means work incomplete; a lot remains to be done both to the theory and the practice.

Every species of organism has tolerance limits with respect to numerous environmental factors. For the sake of concreteness, think of several related species of the marine benthos. Each species has its own specific tolerance limits for temperature and light intensity, to name only two of the (presumably) many environmental factors that control its survival. Considering the effect of a gradient of one of these factors on a mixed community of these species, the relative proportions of the species in a sample would be expected to depend on the level of the gradient at which the sample was taken. And if a batch of samples were taken from various levels, the within-level variation in species composition would be less than the between-level variation.

Next suppose that we wish to compare the relative importance of two environmental factors. As before, let these factors be temperature and light intensity, and imagine an idealized north-south coastline where the following conditions obtain: there is a strong latitudinal gradient in temperature and, at right angles to it, a steep east-west depth gradient and, hence, a strong gradient in light intensity at the bottom. We can now ask which of the two factors, temperature or light intensity, dominates in controlling community composition (this is a conceptual experiment and we choose to disregard all the other varying factors). By sampling at an array of sampling stations so that we have samples from a sequence of depths in each latitude and from a sequence of latitudes at each depth, the necessary data for a straightforward multivariate analysis of variance could (in theory) be obtained.

However, ecological sampling rarely is straightforward, and ambitious plans often turn out to be impracticable. In particular, measurements of species quantities seldom inspire confidence, and tests using ranks are therefore often more appropriate than those depending on absolute measurements. A "natural" way to perform the comparison described above (natural in that it would occur to anyone with a taste for nonparametric statistics) would therefore be to use as data the ranks of the species in each of the samples. Suppose a total of nd regularly arrayed stations have been sampled, at n latitudes and d depths, and the quantities of the same k species are ranked for each sample. Then the data can be displayed as an $n \times d$ table in which each cell contains a list of the ranks of the k species. For instance, if $k=3$, the table would appear thus:



The coefficients of concordance of the rankings within each of the rows, say $W_{1.}, \ldots, W_{n.}$, are now computed; likewise, the concordances of the rankings in each of the columns, $W_{.1}, \ldots, W_{.d}$. (For computational details see, for example, References 1 and 5). We do not enquire whether any of these concordances differ significantly from zero. Almost certainly all of them will. But we do enquire whether the within-latitude concordances tend to differ from the within-depth concordances. If, for example, the within-depth concordances tended to be the greater, we should infer that light intensity influenced community composition (and hence the success of the component species) more strongly than temperature.

The test one is tempted to use to compare the two sets of concordances is the Mann-Whitney test. But, strictly, it is a test for two independent samples and obviously the values of $W_{i.}$ $(i = 1,\ldots, n)$ and $W_{.j}$ $(j = 1,\ldots, d)$ are not independent since each set is based on all nd rankings in the table. I do not know whether the Mann-Whiney test is robust enough for this not to matter. The desired comparison is, indeed, difficult to make. It is difficult enough to compare two coefficients of concordance, that is, two individual values of W, let alone two interdependent sets of W's. Li and Schucany[2] (and see Schucany and Frawley,[4]) described a test to compare two independent values of W. Their test statistic, $\mathcal{W}$, takes values in the range $[-1, +1]$. If concordance is perfect within each set and also the two sets concord exactly with each other, then $\mathcal{W} = +1$; if concordance is perfect within each set and the two sets discord totally with each other (so that the ranking in one set of lists is the exact opposite of the ranking in the other) then $\mathcal{W} = -1$. However, values of $\mathcal{W}$ close to zero are ambiguous; they imply either that one (or both) of the sets has poor internal concordance; or else that, though concordance is good within each set, the two sets are somewhat (not totally) discordant. This latter state of affairs is the one most likely to crop up in the ecological context we are considering. And, as the foregoing discussion suggests, it may prove difficult to diagnose.

Another, and perhaps more important, difficulty that arises is that when a community occupying a gradient is examined it is usually found that as one goes down the gradient, "upslope" species successively disappear and at the same time a succession of "downslope" species are encountered for the first time. If the abundance of the same k species have to be ranked at each station to enable a test to be done, then only a short segment of the gradient can be studied. The same set of k species will not be found in distant samples.

This raises in acute form a conundrum often faced by ecologists concerned with presences and absences of species. Present species can be ranked but not absent ones, though one is often justified in feeling that some are more absent than others. At any point on a gradient a species whose zone starts nearby is "less absent" than one whose zone starts farther away. And besides having magnitude, an absent species' degree of absence from a point should have a sign that depends on whether its presence (its zone) is upslope or downslope from the point.

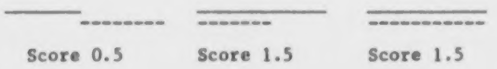
At this stage, speculation must (temporarily) stop. The analysis of ecological data from environmental gradients obviously has much to offer, both to statisticians devising methods and to ecological modelers searching for information on how species in nature do, in fact, react to environmental factors and to one another.

Examples

To exemplify the methods described in the two previous sections, data from Phleger[3] are used. He gives lists of the percentages of different foraminifera species (living and dead) in bottom samples collected at stations at different depths along 12 traverses across the continental shelf in the Gulf of Mexico. The number of stations per traverse ranged from 25 to 55.

Overlap Scores Within Genera

For benthic organisms, zones are not visible, of course. Therefore the zone of any one species was estimated to begin at the shallowest station where it was found and end at the deepest station. It was hoped that because of the large number of traverses errors of estimation in individual traverses would have negligible effect. Small overlaps might chance to go undetected but such errors would tend to be offset by "accidental" specimens occurring outside their zones. Since observations were necessarily discrete, "ties" were possible and were scored thus:



(The method of portrayal corresponds with that in the section, Competing Species and Overlapping Zones.)

All genera with three or more species in at least ten of the traverses were tested to ascertain whether there was any reason to reject the null hypothesis that their zone boundaries were randomly and independently located. The two alternatives were that the zones might show excessively low, or excessively high, overlap. Results for three genera are tabulated below. The two columns for each genus show k, the number of species of the genus in the traverse named (by a Roman numeral) on the left, and the standardized overlap score $L^* = (L-E(L|k))/\sqrt{Var(L|k)}$. With data from 12 traverses available, values of L need not be tested individually. It is clear that the species in the genera Cassidulina and Elphidium show too much overlap for the null hypothesis to be acceptable, whereas for Cibicides it is acceptable. It should be noticed that (disregarding type II errors) the null hypothesis may be found acceptable either because departures from it are insignificant, or because they are indeterminate. The latter will happen if the traverses are too short to go beyond the shallowest and deepest zone boundaries of many of the species; their apparent boundaries will then be randomly ordered.

Table 2. Values of k and L* for Three Genera in Twelve Traverses

Traverse	Cassidulina		Elphidium		Cibicides	
	k	L*	k	L*	k	L*
I	4	0.61	3	0.92	6	0
II	5	1.92	3	0.92	5	0.41
III	5	1.92	3	0.61	8	0.53
IV	5	2.05	4	1.74	8	-0.47
V	5	1.64	4	1.36	9	-0.06
VI	2	1.23	4	1.55	6	-0.21
VII	5	2.33	4	1.36	9	-0.78
VIII	5	1.92	4	0.97	8	0
IX	5	2.60	4	1.16	8	-0.73
X	5	1.23	4	1.36	8	0.07
XI	5	0.68	2	0.61	8	-0.60
XII	4	-0.41	2	0.61	6	-1.04

Concordances of Ranked Species Abundance Lists

The relative abundances of eight common species† (chosen to serve as "community indicators") in samples from three traverses at four depths were listed. The table below shows the traverse numbers (roman) as row labels, the depth ranges as column labels, and values of $W_{i.}$ and $W_{.j}$ to the right of and below the relevant rows and columns. The three entries in each cell of the table are, from top to bottom, the station number where the sample was collected, the depth at that station in meters, and the number of foram tests in the sample. As may be seen from the values of $W_{i.}$ and $W_{.j}$, there is no reason to suppose that community composition varied more with depth than with the horizontal distance between traverses. The traverses did not sample different latitudes; they extended roughly southwards from the Gulf coast of Louisiana and Texas. Even so, the concordances among species rankings from the same depth did not, so far as this small sample shows, tend to exceed the concordances among rankings from different depths on one traverse. With only four traverses and three depths (and these covering only a small depth range) a significant difference would be unlikely to appear in any case; the example is given here merely for illustration. Consideration of only a small range of depths was necessary to ensure that never fewer than six of the eight species chosen as "community indicators" were present in a sample. For the method to be applied over a larger range of depths, a means of scoring absent species objectively must be devised. This is the direction that the work will take next.

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†The species: Bolivina lowmani, B.simplex, Cibicides concentricus, Elphidium discoidale, E.gunteri var galvestonense, Proteonina comprima, P.difflugiformis, Rotalia beccarii var parkinsoniana, Virgulina pontoni. The names given here are those in Phleger's[3] memoir. Name changes resulting from taxonomic revisions have been ignored to facilitate consultation of the original data.

Table 3. Concordances of Species' Ranks Among Samples Grouped by Depths and by Traverses

	Depths				
	22-27m	28-32m	33-37m	38-42m	
VI	#97 22m 350	#101 29m 300	#105 33m 4300	#111 38m 1550	$W_{1.}$ = 0.665
VIII	#380 27m 2000	#378 31m 400	#375 35m 2300	#373 40m 4800	$W_{2.}$ = 0.678
X	#411 26m 1300	#418 29m 3200	#420 35m 5400	#424 42m 250	$W_{3.}$ = 0.751
	$W_{.1}$ = 0.887	$W_{.2}$ = 0.425	$W_{.3}$ = 0.860	$W_{.4}$ = 0.590	

Acknowledgements

I thank Eric Robinson, University of Sydney, Australia, for help with computer programming, and Anita Williams, Halifax, for help with data collation. The work was funded by a grant from the National Research Council of Canada.

Added Note: Dr. F. B. Phleger of the Scripps Institution of Oceanography revised names of the foram species listed in the footnote in the last section. A complete list of names is, in the same order as in the footnote: *Bolivina lowmani*, *B. ordinaria*, *Hanzawaia strattani*, *Cellanthus discoidale*, *Elphidium gunteri*, *Nouria polymorphinoides*, *Reophax difflugiformis*, *Ammonia beccarii* var *parkinsoniana*, *Fursenkoina pontoni*.

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TIME SERIES ANALYSIS AND FORECASTING FOR AIR POLLUTION CONCENTRATIONS WITH SEASONAL VARIATIONS

Der-Ann Hsu and J. Stuart Hunter
Department of Civil Engineering
School of Engineering and Applied Science
Princeton University
Princeton, New Jersey

ABSTRACT

Annual time series records of daily averages of hourly sulfur dioxide concentrations recorded over several major cities exhibit strong seasonal patterns in both level and variation. To construct models useful for prediction and analysis, a Box-Cox transformation is first employed to stabilize the data variability. The transformed data provides a dramatic improvement in the data plots. Further, the transformed data are readily modeled using simple seasonal plus stochastic components following Box-Jenkins time series methods. The fitted models, forecasts and confidence limits are then constructed.

New statistical comparison techniques to compare the stochastic structure of the time series in periods before and after changes in pollution regulations are briefly discussed. These procedures should prove useful in the evaluation of environmental policies.

INTRODUCTION

In this paper, as an illustration of some useful statistical techniques, we analyze twelve annual series of air pollution SO_2 concentrations, collected over four cities: Chicago, Philadelphia, St. Louis and Washington, D.C. All of the series exhibit strong seasonal patterns in both the level and variance. A Box-Cox transformation [1] is first used to stabilize the variances. The transformed data are then fitted by a cosine curve to model the seasonal influences and, following the techniques suggested by Box and Jenkins [2], a stochastic model fitted to account for the day to day time dependent character of the data. Parameter estimates for each of the twelve annual series are provided.

An illustration of forecasting for Chicago SO_2 concentrations using the fitted model is further demonstrated.

In the later part of this paper some techniques useful for comparison of time series are briefly sketched. Potential applications of these methods in the evaluation of environment policies are suggested, and further references furnished.

THE DATA AND THEIR SEASONAL STRUCTURE

Data on SO_2 concentrations were collected from four major cities in the U.S. during the three year period 1969-71. The data consist of hourly readings of the SO_2 concentration for each of the twenty-four hours of a day, measured in units of 0.01 ppm. Although instrument breakdowns, failures of the measuring process, and the negligible levels of concentration during the summer months caused approximately 15% of the readings to be missing, daily averages were computed based upon the available readings within days. A time series plot of the daily averages of SO_2 concentrations in Chicago during 1969, typical of all the series obtained, is displayed in Figure 1.

As can be seen from Figure 1, both the level and the variation are large during the winter and small during the summer. Reasons for these changes are the vast amounts of SO_2 released from household heating systems in the winter, and the different diffusion characteristics due to seasonal temperatures. Over short periods of time, the data also demonstrate skewness towards high SO_2 values.

The failure of the observations to possess a Normal distribution, and/or a homogeneous variance, seriously impedes the ability of the engineer and statistician to postulate models, and to estimate the parameters in these models. For this reason, the Box-Cox transformation[1] was applied to the SO_2 data to enhance Normality, to stabilize the variance, and thus improve the modelling and estimation procedures.

For a variable y, the transformation is expressed as $z^{(\lambda)}$ where

$$z^{(\lambda)} = \begin{cases} \dfrac{(y+\lambda_2)^{\lambda_1} - 1}{\lambda_1 [gm(y+\lambda_2)]^{\lambda_1 - 1}}, & (\lambda_1 \neq 0) \\ gm(y+\lambda_2)\log(y+\lambda_2), & (\lambda_1 = 0) \end{cases} \qquad (1)$$

and

$$gm(y+\lambda_2) = \left[\prod_{i=1}^{n} (y_i+\lambda_2)\right]^{1/n}$$

where n is the number of observations of the variable y and gm is the geometric mean. It has been shown by Box and Cox that the estimates of λ_1 and λ_2, the parameters required in the transformation, can be obtained by minimizing the sum of squares of the residuals after fitting a model. In the present case, the model is a cosine curve, illustrative of seasonal changes in the response level and given by

$$c_t = \beta_o + \beta_1 \cos(2\pi t/365+\alpha), \quad t=1,2,\ldots,365, \qquad (2)$$

where t is the ordinal number of the days within the year and α is the phase angle indicating the starting location of the cosine curve. The model can thus be expressed as

$$z_t^{(\lambda)} = c_t + e_t \qquad (3)$$

where $z_t^{(\lambda)}$, is the Normal variance-stabilized series of the observed SO_2 concentrations. The series of residuals $\{e_t\}$, may be serially correlated, as discussed in a later section.

The estimation of the various parameters in Equations (1) and (2), i.e. λ_1, λ_2, α, β_o, β_1, requires a set of values which minimize $\sum_{t=1}^{365} e_t^2$. Many published computer programs are useful for determining this minimum point (e.g. the subroutine ZXPOWL in the

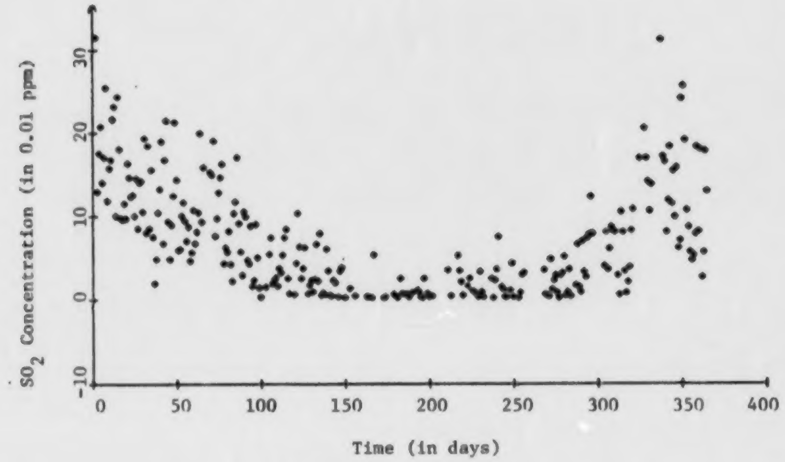

FIGURE 1. OBSERVED DAILY SO$_2$ CONCENTRATIONS IN CHICAGO FOR THE YEAR 1969

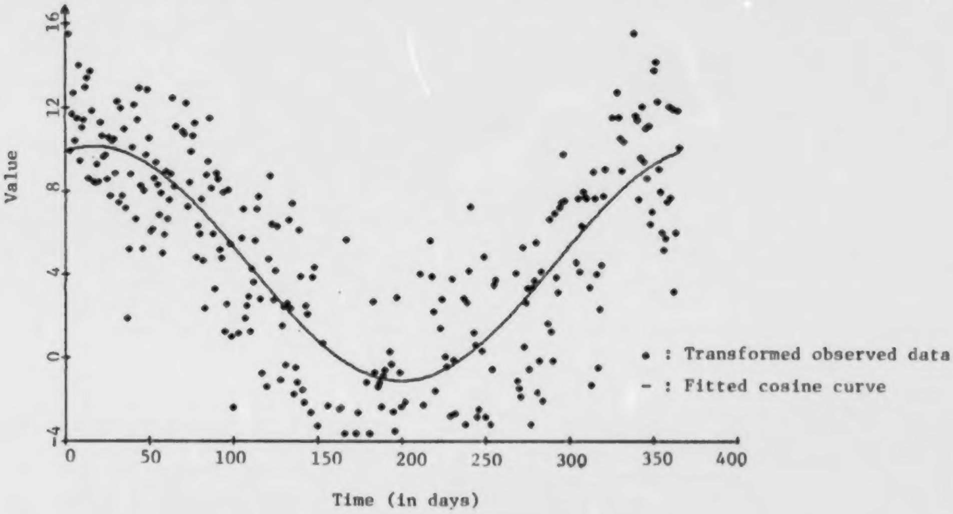

FIGURE 2. THE TRANSFORMED DAILY SO$_2$ CONCENTRATIONS IN CHICAGO FOR THE YEAR 1969 AND A FITTED COSINE CURVE.

IBM's IMSL package). Again, as an illustration, the estimated parameters for the 1969 Chicago data are as follows:

$$\hat{\lambda}_1 = 0.29,\ \hat{\lambda}_2 = 0.00,\ \hat{\alpha} = -.29,\ \hat{\beta}_0 = 4.43,\ \hat{\beta}_1=5.63.$$

Using this set of estimates, the transformed observed data and fitted cosine curve are displayed in Figure 2. The remarkable performance of the transformation in both stabilizing the variance and in elucidating the model is readily seen from the plot.

Similar parameter estimates were obtained for the remaining annual series for the other cities and years. The results are reported in Table 1. Some features of the results are worth commentary. First, all but one estimate of α (the phase angle) falls within the range -.64 to .33 indicating the association between the winter and the high level of SO$_2$ concentration. Second, all but one of the estimates of the transformation parameter λ_2 are negligible, revealing that a transformation with $\lambda_2 = 0$ is adequate in general. Third, the estimates of λ_1 fall between 0.00, (the logarithm transform) and 0.33, (a cube root transform).

THE MODEL FOR THE RESIDUALS

No modelling is complete without an investigation of the residuals. As part of this investigation the sample lagged autocorrelation coefficients, r_k for each of the twelve series were computed using the residuals from the fitted model, where

$$r_k = \frac{\sum_{t=k+1}^{365} (e_t - \bar{e})(e_{t-k} - \bar{e}) \;/m}{\sum_{t=1}^{365} (e_t - \bar{e})^2 \;/\; n}$$

and where m and n are the number of available residuals involved in the calculations, and $\bar{e}$ is the average of the series $\{e_t\}$. Here $\bar{e}$ equals zero. The first ten values of r_k, i.e. $r_1, \ldots, r_{10}$ for the 1969 Chicago data are: (.26, -.03, -.02, .08, .07, .04, .11, .10,

TABLE 1. ESTIMATES OF THE PARAMETERS IN THE MODEL FOR DAILY SO_2 CONCENTRATIONS

City	Year	# Obs.*	$\hat{\alpha}$	$\hat{\lambda}_1$	$\hat{\lambda}_2$	$\hat{\beta}_0$	$\hat{\beta}_1$	$gm(y+\hat{\lambda}_2)$	SSR**	$\hat{\rho}_1$	$\hat{\theta}$	$\hat{\sigma}^2_a$
Chicago	1969	272	-0.2911	0.2857	0.0000	4.4295	5.6257	3.883	2304.4158	0.2605	-0.2811	7.8518
	1970	273	-0.5791	0.0882	0.0000	1.6039	3.8816	2.263	815.7686	0.2641	-0.2856	2.7627
	1971	196	-0.5703	0.1952	0.0000	1.3642	3.9261	2.783	1000.3269	0.4626	-0.6707	3.5202
Philadelphia	1969	226	0.1902	0.0208	0.0000	2.4258	1.0056	2.627	865.5786	0.1651	-0.1699	3.7226
	1970	313	-0.6367	0.1928	0.0021	3.8179	1.4788	3.340	1998.3765	0.3030	-0.3375	5.7317
	1971	284	-0.1887	0.2587	0.0000	1.9199	0.1773	2.303	869.4617	0.3749	-0.4512	2.5436
St.Louis	1969	289	-0.3646	0.3168	0.0000	2.8203	0.2137	2.822	1521.6904	0.4375	-0.5896	3.9072
	1970	236	0.3229	0.2571	0.0000	1.7968	0.2833	2.281	779.0459	0.2797	-0.3059	3.0186
	1971	314	-2.0339	0.0563	0.0000	0.7458	0.4240	1.616	477.5051	0.3528	-0.4130	1.2992
Washington D.C.	1969	283	-0.3215	0.2764	0.0000	1.0519	1.6009	1.609	183.3711	0.3038	-0.3386	0.5813
	1970	270	-0.3170	0.2597	0.0000	0.4850	1.0057	1.320	232.9175	0.3790	-0.4588	0.7127
	1971	326	-0.3914	0.1106	0.7438	3.2043	1.5680	3.019	255.6146	0.2721	-0.2959	0.7210

*The number of observations used in estimation.

**The sum of squares of residuals, $\sum_{t=1}^{n} e_t^2$, after fitting a cosine curve to the transformed observed series.

.02, .03). Following Box and Jenkins[2], this autocorrelation function suggests that, since only the first value is significantly larger than zero at the .05 level, an appropriate model for $\{e_t\}$ is the moving average model of the first order. Thus we have

$$e_t = \mu + a_t - \theta\, a_{t-1} \quad , \; t=2,3,\ldots,365 \tag{4}$$

where a_t are assumed to be independent, identically distributed Normal variables with zero mean and constant variance, μ is the mean of e_t and θ is the moving average parameter. It has been shown that for a such model the theoretical first lagged autocorrelation coefficient, denoted by ρ_1, can be expressed in terms of the moving average parameter θ as follows:

$$\rho_1 = \frac{-\theta}{1 + \theta^2} \tag{5}$$

In practice, the value of ρ_1 is replaced by its sample value and an initial estimate of θ obtained by solving Equation (5) for θ. To confine the solutions to a so-called invertability condition [2, Chapter 3], the absolute value of θ should be less than 1. Only one of the two solutions of θ, based on Equation (5), satisfies this condition. For the 1969 Chicago data, the value of θ was estimated to be -.28.

In addition, the variance of e_t, denoted by σ_e^2 can be expressed as

$$\sigma_e^2 = (1 + \theta^2)\, \sigma_a^2 \tag{6}$$

where σ_a^2 is the variance of a_t. Since the value of σ_e^2 can be estimated from $\{e_t\}$, given the value of θ, we may estimate σ_a^2 based on Equation (6). For the example in hand we have $\hat{\sigma}_e^2 = 2304.42/272 = 8.47$. The value of $\hat{\sigma}_a^2$ is thus equal to $8.47/[1+(.28)^2] = 7.85$, assuming $\theta = -.28$.

Parameter estimates for the residuals of other annual series of daily averages of SO_2 concentrations were also obtained and are displayed in the last two columns of Table 1. The values of $\hat{\theta}$ fall between -.59 and -.17 indicating that a significant positive correlation exists between the concentrations of immediately consecutive days (see Equation (5); a negative θ corresponds to a positive ρ_1). The values of $\hat{\sigma}_a^2$ are not comparable among series since individual transformations were applied to each series.

FORECASTING OF THE CONCENTRATIONS

Forecasting is important in all time series modeling, both as a check on the adequacy of the model as a description of a system, and for the purpose of control of the system. From the models fitted in previous sections, forecasts of the SO_2 concentrations for a moderate length of time ahead can be obtained. The first stage of determining forecasts is to predict the values of e_t at time T+1, T+2, ..., assuming that we stand at time T, the time origin of prediction. Again, as suggested by Box and Jenkins, the best forecasts of e_{T+k}, k=1,2,... are

$$\begin{aligned} \hat{e}_{T+1} &= \bar{e} - \theta\,\hat{a}_T \\ \text{and} \quad \hat{e}_{T+k} &= \bar{e} \qquad \text{for } k \geq 2 \end{aligned} \tag{7}$$

where $\hat{a}_T$ can be obtained by fitting the model expressed by Equation (4) to the observed series of e_t. The value of $\bar{e}$ in this case is equal to zero. The upper and lower bounds, at the .95 confidence level, of the forecasts can be computed following the equations displayed below:

$$\begin{aligned} \hat{e}_{T+1} \pm \varepsilon_{T+1} &= \hat{e}_{T+1} \pm 1.96\,\hat{\sigma}_a \\ \hat{e}_{T+k} \pm \varepsilon_{T+k} &= \hat{e}_{T+k} \pm 1.96\,\hat{\sigma}_a\,(1+\theta^2)^{\frac{1}{2}} \text{ for } k \geq 2 \end{aligned} \tag{8}$$

where ε's indicate half the length of the confidence intervals.

To express the forecasts in the original form and scale, a seasonalization and reverse variance-stabilizing transformation is made where

$$\hat{z}^{(\lambda)}_{T+k} = \hat{\beta}_o + \hat{\beta}_1 \cos[2\pi(T+k)/365 + \hat{\alpha}] + \hat{e}_{T+k}\ , k\geq 1 \tag{9}$$

$$\text{and} \quad \hat{y}_{T+k} = \{\hat{z}^{(\lambda)}_{T+k}\,\hat{\lambda}_1\,[gm(y_t + \hat{\lambda}_2)]^{\hat{\lambda}_1 - 1} + 1\}^{1/\hat{\lambda}_1} + \hat{\lambda}_2 \tag{10}$$

The confidence limits of y_{T+k} are secured by adding or subtracting from Equation (9) an ε_{T+k} already defined and then going through the procedure expressed in Equation (10). Using the Chicago example the daily averages of SO_2 concentrations for the first hundred days of 1970 are displayed in Figure 3. The forecast which is the expected median of future realizations of SO_2 concentration at time T+k and its associated upper and lower 2.5% probability limits are also displayed in Figure 3. The observed concentrations fall within the forecast confidence band in a fashion very consistent with theoretical expectation.

In viewing Figure 3, it is important to remember that the probability density in the original metric of the observations appears skewed to the upper side and further, that the variance is not independent of level. In addition, it is interesting to note the tendency of the observations to gradually drift below the forecast line near the end of the 100 day series. We have here an indication of the possible inadequacy of the forecast function and are led naturally to the question of comparing the 1969 and 1970 models.

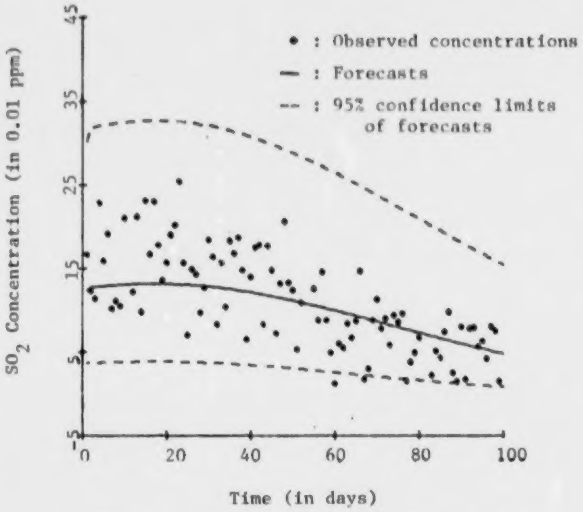

FIGURE 3. FORECASTING SO_2 CONCENTRATIONS IN CHICAGO FOR THE FIRST HUNDRED DAYS OF 1970.

COMPARISON OF TIME SERIES

Besides forecasting, the comparison of time series is an important problem in applied statistics. Situations which require comparison of time series may arise when the effects of, say, changes of pollution regulations are to be assessed. The time series of pollution concentrations before and after the regulation changes, for instance, may be investigated and compared with respect to such essential features as their overall level, autocorrelation structure, variation and the probability of exceeding some regulatory standard (or the frequency of occurrence and duration of excedences of a regulatory standard).

Comparison through the use of forecasts. A simple method to test whether two time series have identical structure is to perform forecasting for one series (series B), using the model constructed from the other (series A). The differences between the forecasted and observed values for series B can be tested for potential model discrepancy. Tiao, Box and Hamming[5] proposed that the errors of one-step-ahead-forecasts, i.e. $\hat{a}_{T+k}$, k=1,2,3,..., be squared and summed and then checked against the significance point of a χ^2 distribution, given that Normality may be assumed for the errors.

In the case of SO_2 concentrations, the fitted model including the estimates of λ_1, λ_2, α, β_o, β_1 and θ, for the A series can be used to obtain forecasts for B series. If the parameters are different between the two series the corresponding forecast errors will exhibit a systematic bias, or a structured stochastic pattern. An illustration of this comparison technique is not shown in this paper, but is under current study.

Comparison using a test statistic for Normal stationary models. A test statistic for comparing two autoregressive time series has been developed by Hsu[3] and illustrated in a practical example by Hsu and Hunter[4]. This technique is useful for comparing two series of residuals with respect to parameters θ and σ^2_a.

Comparison using a complete test. Ideally, a test statistic or scheme can be developed to examine all the parameters of two series. Such a test, which promises to be complicated and to require much computation is left for future research.

CONCLUDING REMARKS

Series of daily averages of SO_2 concentrations have been analyzed to demonstrate a profitable use of some statistical techniques. Data which originally appeared to be lacking a simple structure were variance-stabilized, deseasonalized and fitted by a simple stochastic model. Forecasts of future levels of pollution concentrations were easily obtained using the fitted model. Further, series observed from different locales could be compared based on the information gathered from their analyses and models. Activities such as evaluation of environmental policies, selection of alternative regulations, etc., may thus benefit from such studies. Further, analyses of hourly data within a day are also possible and may be expected to provide valuable information. Geographical comparison, combinations of statistical and physical models, schemes adaptive to pollution control, etc., are all subjects for further investigation. The authors hope the statistical techniques described here may prove useful in these future research activities.

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METEOROLOGICAL ADJUSTMENT OF YEARLY MEAN VALUES FOR AIR POLLUTANT CONCENTRATION COMPARISONS

Steven M. Sidik
NASA-Lewis Research Center
Cleveland, Ohio

Harold E. Neustadter
NASA-Lewis Research Center
Cleveland, Ohio

Summary

The results of some linear regression analyses relating pollutant concentrations to certain specified meteorologic and economic variables are presented. The resulting models provide about a 20 percent improvement in predicting concentrations. An outline of the use of the predictive equations in adjusting for meteorological effects is then presented.

Introduction

This paper presents an approach to interpretation of 24-hour averaged air pollutant measurements taken in compliance with U. S. Environmental Protection Agency guidelines when analyzed in conjunction with such meteorological data as may be readily obtained from the National Weather Service. The specific example considered is Total Suspended Particulates in Cleveland, Ohio, for which some monitoring has been performed by the municipality since 1967; initially every 6th day and currently every 3rd day. The meteorological data are also for the same 24-hour periods and was obtained from National Oceanic and Atmospheric Agency as decks of punched cards. The information is ground level information and devoid of such things as inversion heights.

We fit linear regression models to pollutant concentrations using the following combinations of meteorologic variables as predictors: daily delta temperature (defined as the maximum temperature minus the minimum) and its first difference; daily minimum temperature and its first and second differences; daily average barometric pressure; daily total precipitation (water equivalent in inches); and daily resultant wind velocity. We included two rough indicators of economic activity and allowed for the existence of both a linear "drift" in time and a seasonal component with a period of 1 year.

The overall results are that the mean TSP concentration (1) increases as delta temperature increases and as its first difference decreases; (2) increases as minimum temperature increases and as the first and second differences increase; (3) increases as pressure increases; (4) generally decreases initially with increasing wind velocity except when there is a source upwind; and (5) significantly decreased over the period of the study with a clear indication of seasonal fluctuation.

The goodness of fit of the estimated models to the data is partially reflected by the squared coefficient of multiple correlation, indicating that at the various sampling stations the models accounted for about 23 to 47 percent of the total variance of observed TSP concentrations. However, there is still a large variability unaccounted for so that predictions of individual values are not very helpful.

About a 20 percent improvement when using these equations in place of simple mean observed values is obtained when (1) predicting mean concentrations for specified meteorological conditions or (2) comparing yearly averages after being adjusted so as to remove meteorological effects.

Pollutant Concentration Data

The Cleveland Division of Air Pollution Control has taken 24-hour averaged air quality samplings of TSP since January 1967. There are currently 21 sampling stations around the city which sample TSP. A more complete analysis of all these stations (including analysis of SO_2 and NO_2 data) is presented elsewhere.[1] Only a summary of the results for TSP is included herein and illustrated by the results from a typical station.

Summaries of the air pollution data used for this study, including tabulations of means, standard deviations and goodness of fit to lognormality on an annual basis have been reported earlier.[2]

The sampling method for TSP is high volume air sampling using Glass fiber filters. A previously published study showed that, for such HiVol air sampling of TSP in Cleveland, approximate 95 percent confidence limits on the errors introduced by filters and samplers were about 12 percent high to 11 percent low.[3]

Regression Analysis

Models and Method

The method chosen for data analysis was multiple linear regression analysis which is explained in such texts as Searle,[4] Draper and Smith,[5] and Daniel and Wood.[6]

We assume models of the general form

$$y_i = \beta_o + \sum_j \beta_j x_{ij} + \epsilon_i \qquad (1)$$

where

y_i the i^{th} observed pollutant concentration, or some transformed value of that concentration. In this paper we use $y = \log(TSP)$

x_{ij} the observed value of the j^{th} predictor variable (i. e., meteorologic economic) for the i^{th} observation. The particular predictor variables (such as barometric pressure) used are presented in Table 1

β_o the unknown intercept values

β_j unknown coefficients (slopes) which are to be estimated. Multiple linear regression as used here estimates these unknown coefficients by the method of least squares. (Estimated values are denoted by $\hat{\beta}_j$)

ϵ_i an unobserved random error component. This random error is assumed to follow a normal distribution with mean of zero and a standard deviation of σ which is unknown. We further assume that the ϵ_i are uncorrelated with each other

The random error ϵ_i will include, among other things, errors of measurement of the concentrations, inherent variability of concentration because of varying emission rates and/or atmospheric instability, inadequacies in the model, and to some extent the errors of measurement of the predictor variables. Our data base consists primarily of 24-hour averaged concentrations at 3 day intervals. A previous study[7] found that concentrations observed every 3 days have a very low correlation. Thus the assumption that the ϵ_i are uncorrelated is reasonable.

Derived Variables and Estimated Coefficients

Pollutant concentrations at a given time and location are the result of emissions from various sources which have undergone transport and dispersion processes in the atmosphere. In general, for a fixed rate of emission from all sources, pollutant concentrations are inversely proportional to atmospheric mixing. The factors generally considered to control the degree of mixing are the effective mixing height, wind velocity, and wind stability.[8] In most locations, however, the NWS does not routinely monitor mixing heights. Thus, this information has not been incorporated even though such measurements were made locally by the NWS for a period of 1 year.

To construct model equations which can predict pollutant concentrations for known meteorological conditions, we defined new predictor variables derived from those basic variables known or suspected to be related to atmospheric mixing. In constructing derived variables we were guided primarily by Holzworth's[9] qualitative account of large scale weather influences on air pollution concentrations.

Table 1 presents the 29 derived variables used in the predictive models. These variables, the rationale for their inclusion and the results are discussed in depth in Ref. 1. This model was fitted separately at each station. Due to space limitations, we present the results of the regression analysis at only one of the sampling stations. Full analysis is presented in Ref. 1. The chosen station is typical in the sense that it falls approximately in the middle of the range of how well the equations fit the data.

Table 2 presents (1) the estimated coefficients for each predictor variable, (2) the value of square of multiple correlation coefficient (R^2), (3) the number of observations available for fitting, (4) the estimate of the error variance ($\hat{\sigma}^2$) and error standard deviation ($\hat{\sigma}$), and (5) the mean of the observed concentrations ($\bar{y}$). The meaning and use of each of these quantities are discussed in the following sections.

Goodness of Fit and Error Estimate

Table 2 of Ref. 1 shows that for TSP the R^2 values range from a low of 0.23 to a high of 0.47 with most of the values near 0.40. In other words, the models account for from 23 to 47 percent of the total variance of the log(TSP) values.

Table 2 of Ref. 1 also shows that, for log(TSP), $\hat{\sigma}$ ranges from 0.140 to 0.233 with most values being around 0.160. The importance of $\hat{\sigma}$ to the problem of using the models to predict concentrations will be covered in the following section.

Applications

Predictions from Fitted Models

The primary motivation of this work was to develop a method for making predictions. Actually, two different predictions are of interest. The first is the prediction (or estimate) of the mean pollutant concentration as a function of the predictor variables and the second is the prediction of a single further pollutant concentration. Both predictions results from inserting the specified values of the predictor variables (i.e., the x_j) into the estimating equation yielding

$$\hat{y} = \hat{\beta}_0 + \sum \hat{\beta}_j x_j$$

However, the uncertainties (standard deviations) associated with each application are different.

The uncertainty in the prediction of the mean of the y's for specified x_j is a function only of the actual x_j and the uncertainty of the estimates $\hat{\beta}_j$. (See Draper and Smith[5] and Hahn[10] for details. We consider predictions only at the means of the x_j for notational and conceptual simplicity.) The estimated standard deviation of $\hat{y}$ when the x_j are all equal to the means of the x_j is $\hat{\sigma}/\sqrt{N}$. For the TSP data of station 1 we obtain a standard deviation of $0.176/\sqrt{364} = 0.0092$. Thus an approximate 95 percent confidence limit on y is

$$\hat{y} - (1.96)(0.0092) \le \log(\mathrm{TSP}) \le \hat{y} + (1.96)(0.0092)$$

In terms of TSP directly this results in proportional limits of

$$10^{\pm(1.96)(0.0092)} = (1.04, 0.96)$$

or roughly ±4 percent. Thus the regression equation itself is pretty well estimated. These confidence limits change as the x_j change.

The uncertainty in a further predicted value includes not only the uncertainty in the regression equation but also the uncertainty involved in a single observation. The standard deviation of a further predicted value at the mean of the predictor variables is thus

$$\hat{\sigma}\sqrt{1+\frac{1}{N}}$$

At station 1 for log(TSP) we thus obtain 0.1762.

Approximate 95 percent confidence limits (in terms of proportional limits) thus becomes

$$10^{\pm(1.96)(0.1762)} = (2.22, 0.45)$$

That is we can predict single values with a 95 percent confidence of being within 55 percent low to 122 percent high. Thus although the regression function is well estimated, it is obvious that it is practically useless for prediction of specific single day concentrations because of the large residual error. We will now consider a situation where the regression equation can be used to advantage.

Use in Meteorological Adjustment

The previous section showed that the large residual variability precluded meaningful individual predictions of concentrations. Nevertheless, if many concentrations are predicted and then averaged, the average concentration can be estimated with dramatically improved reliability.

Suppose we use the current predictive models for a period of say 1 year and that during this year we accumulate $N = 100$ further observations. Among other differences between this year and previous years are the differences in meteorological conditions on the days for which data was obtained. If we assume that measured concentrations are related to emission rates and we want to compare the emission rates of this year with those of previous years based on the changes in measured concentrations, then it is necessary to first remove (adjust for) these meteorological differences. This is accomplished by computing the estimated deviations

$$\hat{\epsilon}_i = y_i - \hat{y}_i$$

of the predicted concentrations ($\hat{y}_i$) from the observed (y_i) values. If there have been no changes in the processes generating the pollutants then the predicted and the observed concentrations should be the same on the average. That is, the $\hat{\epsilon}_i$ would ideally have a distribution with a mean of zero and we expect the computed mean, $\bar{\epsilon}$, to be near zero. (Note that the $\hat{\epsilon}_i$ will not have the same variance. See Ref. 5 for details.)

If there has been an increase in emissions, $\bar{\epsilon}$ would tend to be greater than zero, while the opposite would be true if there were a decrease in emissions. Thus a statistical test of the hypothesis of unchanged conditions is equivalent to a test of the significance of the difference of $\bar{\epsilon}$ from zero. The standard deviation of $\bar{\epsilon}$ is related to the standard deviation of $\hat{\epsilon}_i$ by the factor of $1/\sqrt{N}$. Thus, using the log(TSP) data of Table 2 and assuming $N = 100$ observations we obtain an estimated standard deviation of 0.01762 for $\bar{\epsilon}$ which translates to approximately ±8 percent for a 95 percent confidence interval on $\bar{\epsilon}$.

Obviously, as more data became available (e.g., each year) updating of the data base should be done and the models refitted. At these times the models could also be improved by the inclusion of other variables found to be of significance.

Degree of Improvement

We have discussed how well the models fit the data and the use of the models for prediction purposes. We now consider the question of how much improvement we have achieved by using the estimated regressions as opposed to using the mean of the observed concentrations without any adjustment. The quantity $D = 1 - \sqrt{1 - R^2}$, where R^2 is as defined previously (i.e., the square of the multiple correlation coefficient) expresses the proportional decrease in the standard deviation of a predicted concentration when the regression equation is used as opposed to simply using the mean of the observed values. (Duncan,[11] pp. 696-699.)

From the R^2 values of Table 2 of Ref. 1 we find that $D = 1 - \sqrt{1 - R^2}$ ranges from a low of 0.123 to a high of 0.272. Most of the R^2 values are near $R^2 = 0.40$ which gives a value of $D = 0.225$. We thus find a percent improvement of from 12.3 to 27.2 percent with most values near 20 percent.

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TABLE 1. - DERIVED PREDICTOR VARIABLES USED IN THE REGRESSION MODELS

Variable	Symbol	Definition
X_1	ΔT	$T_{max} - T_{min}$; maximum temperature minus temperature, °F
X_2	$\Delta T'$	$+3\,\Delta T_i - 4\,\Delta T_{i-1} + \Delta T_{i-2}$; related to noncentral first difference of ΔT on day i
X_3	min	T_{min}; minimum temperature, °F
X_4	min'	$+3\,\text{min}_i - 4\,\text{min}_{i-1} + \text{min}_{i-2}$; related to noncentral first difference of min on day i
X_5	min''	$-2\,\text{min}_i + 5\,\text{min}_{i-1} - 4\,\text{min}_{i-2} + \text{min}_{i-3}$; related to noncentral second difference of min at day i
X_6	B. P.	Daily average barometric pressure in inches of mercury
X_7	Pr	Total water equivalent of precipitation in inches
X_8	$(\text{Pr})^2$	The square of X_7
X_9	Work	Indicator of workdays vs nonworkdays $\text{Work} = \begin{cases} 0 & \text{Saturday, Sunday, Federal holidays} \\ 1 & \text{Otherwise} \end{cases}$
X_{10}	Steel	Weekly regional steel tonnage index
X_{11}	v_N	$v_N = \begin{cases} \text{Resultant velocity; when wind is out of the North octant} \\ 0.0, \text{ Otherwise} \end{cases}$
X_{12}	v_N^2	X_{11}^2
X_{13}	v_{NE}	Similar to X_{11}, X_{12} when wind is from NE
X_{14}	v_{NE}^2	
X_{15}	v_E	Similar to X_{11}, X_{12} when wind is from E
X_{16}	v_E^2	
X_{17}	v_{SE}	Similar to X_{11}, X_{12} when wind is from SE
X_{18}	v_{SE}^2	
X_{19}	v_S	Similar to X_{11}, X_{12} when wind is from S
X_{20}	v_S^2	
X_{21}	v_{SW}	Similar to X_{11}, X_{12} when wind is from SW
X_{22}	v_{SW}^2	
X_{23}	v_W	Similar to X_{11}, X_{12} when wind is from W
X_{24}	v_W^2	
X_{25}	v_{NW}	Similar to X_{11}, X_{12} when wind is from NW
X_{26}	v_{NW}^2	
X_{27}	t	Number of days from Jan. 1, 1967 divided by 100 (Jan. 1, 1967 is nominal beginning of sampling program)
X_{28}	$\sin(\theta)$	$\sin(2\pi t/3.6525)$
X_{29}	$\cos(\theta)$	$\cos(2\pi t/3.6525)$

TABLE 2. - RESULTS OF REGRESSION ANALYSIS AT A TYPICAL STATION FOR TOTAL SUSPENDED PARTICULATES

Coefficient	Variable	Estimate	Coefficient	Variable	Estimate	Coefficient	Variable	Estimate
β_0	Intercept	-2.91	β_{10}	Steel	-0.00040	β_{20}	v_S^2	0.00042
β_1	ΔT	[a].0080	β_{11}	v_N	[a]-.040	β_{21}	v_{SW}	-.011
β_2	$\Delta T'$	-.00034	β_{12}	v_N^2	.0019	β_{22}	v_{SW}^2	.00008
β_3	min	[a].0033	β_{13}	v_{NE}	[a]-.045	β_{23}	v_W	[a]-.024
β_4	min'	[a].0022	β_{14}	v_{NE}^2	[a].0021	β_{24}	v_W^2	.00099
β_5	min''	[a].0013	β_{15}	v_E	[a]-.070	β_{25}	v_{NW}	[a]-.044
β_6	B. P.	[a].17	β_{16}	v_E^2	[a].0044	β_{26}	v_{NW}^2	[a].0027
β_7	Pr	[a]-.30	β_{17}	v_{SE}	-.027	β_{27}	t	[a]-.0081
β_8	$(Pr)^2$	[a].16	β_{18}	v_{SE}^2	.00065	β_{28}	$\sin\theta$	[a].11
β_9	Work	.016	β_{19}	v_S	[a]-.020	β_{29}	$\cos\theta$	[a].090

[a] Denotes the coefficient is significantly different than zero at approximately the 10 percent significance level.

N	364	$\hat{\sigma}^2$	0.0310
$\overline{Y}$	2.09	$\hat{\sigma}$	0.176
R^2	0.38	D	0.21

THE APPLICATION OF CLUSTER ANALYSIS TO STREAM WATER QUALITY DATA

Jay A. Bloomfield
Environmental Quality Research Unit
New York State Department of Environmental Conservation
50 Wolf Road, Albany, New York 12233

Abstract

Cluster analysis, a multivariate classification technique was used to examine spatial and temporal heterogeneity in stream water quality data. To examine spatial patterns, stream water quality data from 44 watersheds in the Genesee River basin in western New York State were analyzed. Nine groups of watersheds and seven groups of water quality variables were identified. To examine temporal trends, data collected daily at a small rural watershed, Mill Creek, were examined. Three clusters of state variables were produced, based upon the stability of each variable during runoff events. Cluster analysis by sample yielded subsets representing runoff events, recessional periods and base flows.

Introduction

One of the more challenging problems in the environmental sciences today is the interpretation of data collected from field studies. These data often consist of many state variables measured at several locations over a period of time. The sheer volume of data obtained in this manner often overwhelms even the most thorough observer, intent upon discerning meaningful patterns in the data. Several multivariate techniques have been used to find patterns in environmental data, primarily in the fields of geology, taxonomy, and terrestrial ecology. These techniques include multiple components analysis (McCammon, 1968), ordination (Bray and Curtis, 1957) and cluster analysis (Fortier and Solomon, 1966). This paper will be concerned solely with the latter, a hierarchical classification technique used to determine subsets of samples or state variables. Two data sets will be analyzed using cluster analysis: one to examine spatial heterogeneity, and the other to examine temporal variability in stream water quality.

Sources of Heterogeneity in Stream Water Quality Data

Heterogeneity in stream quality is due to two factors, time and location. Temporal variability in water quality is induced by seasonal and short-term changes in climatic factors, primarily precipitation, but to a lesser extent, solar radiation and the movement of air masses. Spatial variability is often explained by differences in soil or bedrock type, topography, vegetation or the influence of the activities of man.

Stream quality surveillance networks are rarely designed to evaluate both spatial and temporal variations in water quality, either because of limited resources or lack of insight. Little effort is made in determining 1) the proper sampling interval, 2) the placement of stations, or 3) redundancy in the state variables (primarily chemical constitutents) measured. Cluster analysis can be used to examine each of these three problem areas.

Cluster Analysis

Cluster analysis is simply a classification technique which graphically describes a similarity matrix with a dendrogram (Sokal and Sneath, 1963). The similarity matrix can be constructed by comparing samples (Q-mode) or state variables (R-mode). For each pair of samples or variables, a similarity coefficient is calculated. Although the correlation coefficient is often used, it has the disadvantage of marked sensitivity to the nature of the frequency distribution of the state populations (variable or sample) considered (Park, 1968; Gevirtz, Park and Friedman, 1971).

A distance coefficient proposed by Sorensen (1948) tends to be less sensitive to the form of the frequency distribution of the data (Park, 1968) and therefore, has been used in this paper.

Sorensen's coefficient (S) for multistate data is defined as:

$$S_{jk} = 2* \frac{\sum_{i=1}^{n} (\text{minimum}\ (X_{ij}, X_{ik}))}{\sum_{i=1}^{n} X_{ij} + \sum_{i=1}^{n} X_{ik}}$$

For Q-mode analysis, n is the number of samples, X_{ij} the value of the jth state variable in the ith sample, and X_{ik} the value of the kth state variable in the ith sample. For R-mode analysis, the logic is transposed. It can be seen that the coefficient represents the relative amount a pair of samples or variables has in common.

The generation of the dendrogram is accomplished by pair-wise calculation of elements of the similarity matrix. From this matrix, the pair of states with the maximum value of S are temporarily deleted from the analysis, and the program recalculates the similarity matrix with an additional state obtained from a combination of the pair of states deleted. Thus, n-1 iterations are required to produce the dendrogram. This step-wise procedure allows one to examine the hierarchy among subsets (King, 1967).

An example of a dendrogram is shown in Figure 2. The horizontal scale represents percent similarity (100. * S). The states are listed vertically and are connected with parallel lines. If states A and B are similar at a 90% level, parallel lines are drawn horizontally to this level and connected. If state C is similar to this subset at a 75% level, parallel lines are extended from the A-B subset (90%) to 75% and are connected to a horizontal line from state C. The simplest procedure for defining a cluster is to compare the relative similarity within a group to the similarity of the group to the remainder of the states.

Gevirtz et al (1971) sites a disadvantage with cluster analysis: the technique produces subsets of states, and hence obscures gradients among states. Additionally, McCammon (1968) has warned to ignore low level clusters ($S < .2$) and Park (1974) has suggested scaling each state variable (either by the maximum value of each variable or the range). Both of these suggestions have been followed in this paper. Also, the author believes the results obtained from cluster analysis should be used judiciously, taking into account the limitations of the data and should function as one facet of a rigorous analytical strategy.

Cluster analysis has been used in geology (Harbaugh and Merriam, 1968), marine biology (Gevirtz et al, 1971), paleoecology (Del Prete, 1972; Bloomfield, 1972) and limnology (Cairns, Kaesler and Patrick, 1970). The technique has application to a wide range of multistate environmental data where grouping of similar states is desired.

Results

Two sets of multivariate stream water quality data were examined using a cluster analysis program written in FORTRAN and described by Gevirtz et al (1971). Each data set was chosen so as to examine the problems of spatial and temporal heterogeneity.

The Genesee River Watershed, 1972

During June 1972, the United States Geological Survey sampled 44 streams in the Genesee River Basin in western New York (Figure 1). Twenty-one water quality parameters including water temperature and stream discharge were determined for each stream (United States Department of the Interior, 1973). On June 23, 1972, Hurricane Agnes, one of the most severe storms ever to affect New York State, caused vastly increased stream discharges. Of the 48 total sampling sites, six were sampled after the storm. Five of these post-storm sites were on the main stem of the Genesee River and one on a major tributary. Cluster analysis was used to group both sampling sites (Q-mode) and state variables (R-mode). The Q-mode dendrogram is shown in Figure 2 and the R-mode dendrogram in Figure 3.

The Q-mode analysis generated nine distinct clusters, four intermediate samples, and one sample (Wolf Creek) that was unique from the other 44 samples. Four samples were not included in the analysis because of missing values for one or more state variables. Two of the clusters (C and D) and two intermediate stations (Genesee River at Wellsville and Avon) account for the six post-storm sampling sites. The remaining cluster (A_1, A_2, A_3, A_4, B, E and F) represent pre-storm sites. The geographical distribution of these clusters is shown in Figure 4. It is apparent that the pre-storm clusters are areally compact, representing regions with similar environmental conditions. Table 1 displays land use, soil quality and bedrock geology for the seven pre-storm clusters.

The A clusters represent a forested region (Hardy and Shelton, 1970) in slightly-coarse textured, moderate to somewhat poorly-drained acidic soils (Cline, 1961) underlain by Upper Devonian shales and siltstones (New York State Education Department, 1970). Cluster B has bedrock geology and soils similar to the A clusters but there are some agricultural areas in the watersheds of this cluster. Clusters E and F represent agricultural watersheds in lime-rich well-drained soils. The watersheds of cluster E are underlain by Devonian shales and limestones while the watersheds of the F cluster are underlain by Upper Silurian shales, dolostones and evaporites.

Examination of the geographic distribution of the Q-mode clusters (Figure 4) would dictate that the unique Wolf Creek sample be a member of cluster B. Inspection of the data from Wolf Creek shows relatively high sodium (600 mg/l) and chloride (1200 mg/l). The apparent reason for the uniqueness of this site is the existence of a large salt mining operation in the Wolf Creek watershed (New York State Department of Health, 1961).

Table 2 summarizes the average value and range of three water quality parameters, chloride, nitrate-nitrogen and alkalinity by Q-mode cluster. Alkalinity, chloride and nitrate are decidedly higher in the agricultural clusters (E and F). Figures 5 through 8 show the geographic distribution of chloride, nitrate-nitrogen alkalinity and electrical conductivity. What causes these trends is most probably a combination of land use, soil type and bedrock geology. An ongoing study (New York State Department of Environmental Conservation, 1974) is attempting to determine which of these three factors is most directly responsible for trends in stream water quality in the Genesee River Basin.

The R-mode analysis resulted in seven groups of water quality variables (Figure 3):

1) Ca^{++}, hardness
2) $SO_4^=$, non-carbonate hardness
3) Dissolved solids, electrical conductivity
4) pH, water temperature, $SiO_3^=$
5) HCO_3^-, alkalinity
6) Stream discharge, total Fe, total Mn
7) Na^+, Cl^-

The composition of several of the R-mode clusters are readily explainable, showing redundancy between state variables. For example, cluster 5 contains alkalinity and HCO_3^-, which is the major component of alkalinity encountered at neutral pH. Cluster 3 contains electrical conductivity and dissolved solids, the concentration of the latter being the major factor in determining the electrical conductivity of an aqueous solution.

Cluster 1 contains hardness and its major constituent calcium. Cluster 6 relates stream discharge, iron and manganese. This cluster results from high iron and manganese in post-storm samples only, possibly related to increased levels of suspended sediment. Cluster 7 probably results from the influence of salt deposits (NaCl) in the watershed. Cluster 2 relates sulfate ion and non-carbonate hardness (polyvalent dissolved cations such as strontium and zinc). Cluster 4 consists of pH, stream temperature and silicate. The author can offer no simple explanation for clusters 2 and 4.

Thus, cluster analysis can be used to examine spatial variation in stream water quality data from the Genesee watershed and has allowed classificiation of seven groups of water quality parameters.

The Mill Creek Watershed, 1975

Eighteen water quality parameters were measured at Mill Creek, New York, for one year beginning March 1, 1975 (Hetling, Carlson and Bloomfield, 1976). The watershed has an area of about 25 km^2 and land use is evenly divided between agriculture and forest (El-Baroudi, James and Walter, 1975). Stream discharge was gaged continuously and one water sample was collected each morning. Additional samples were collected during major runoff events.

Cluster analysis was performed on a data set consisting of the morning samples collected between April 1, 1975 and October 31, 1975 (214 samples). The Q-mode dendrogram is summarized in Figure 9. In general, the samples representing the three major runoff events (April 4, August 8 and October 18) form one cluster (J). Each of these events represent a prolonged stream discharge of over 2.0 m^3/sec. Other clusters represent smaller runoff events D, H), recessional periods immediately following events (A, B, C, E, G, I) or prolonged periods of drought (F). These twelve unique Q-mode clusters account for slightly over one-third of the total number of samples. The remaining samples form a very diffuse cluster of similarity greater than 95%. These samples represent base flow conditions and yield water quality information that is extremely redundant.

The results of the Q-mode analysis suggest more frequent sampling during runoff events with fewer samples during base flow. Anomalous extended dry periods should be sampled more frequently when possible.

The R-mode dendrogram (Figure 10) shows three major clusters of water quality variables:

1) Dissolved organic carbon, dissolved kjeldahl nitrogen, chloride, dissolved orthophosphate phosphorus, total dissolved phosphorus, ammonia nitrogen and nitrate nitrogen.

2) Alkalinity, electrical conductivity, sulfate, pH, dissolved oxygen and nitrate nitrogen.

3) Particulate organic carbon, particulate phosphorus, suspended solids, particulate kjeldahl nitrogen and stream discharge.

Cluster 1 represents dissolved constituents which exhibit changes in concentration during runoff events. Cluster 2 also represents dissolved constituents. However, these variables tend not to be as influenced by runoff events. The constituents in cluster 3 are extremely influenced by runoff events. Cluster 3 includes stream discharge and four particulate (retained on a 0.45 μm membrane filter) variables. In summary, the R-mode analysis indicates that three subsets of water quality variables can be defined based upon their relationship to runoff events.

Conclusions

Cluster analysis can be used to examine spatial and temporal heterogeneity in stream water quality data. It can also be used to check for redundancy among water quality variables.

Analysis of water quality data from the Genesee River Basin indicates that land use and geology tend to be the most significant factors in determining the actual grouping of subwatersheds within the basin. The use of cluster analysis on time-course data from Mill Creek, New York, reveals three subsets of variables; stable dissolved, variable dissolved and extremely variable particulate constituents. Q-mode analysis of the Mill Creek data resulted in grouping samples into runoff event, hydrograph recession and low flow groups. This result tends to agree with the results of Bouldin, Johnson and Lauer (1975) and Hetling, Carlson and Bloomfield (1976) that runoff event-oriented and not fixed-interval sampling yields more reliable data on stream water quality.

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Key to Figure 1

Watersheds sampled prior to Hurricane Agnes

1) Spring Creek (Pumpkin Hill)
2) Black Creek (Churchville)
3) Hotel Creek
4) Mill Creek (West Chili)
5) Spring Creek (Mumford)
6) Pearl Creek
7) Stony Creek
8) Warner Creek
9) Trout Brook
10) Wolf Creek
11) Beards Creek
12) Jaycox Creek
13) Christie Creek
14) White Creek (Canawaugus)
15) Dugan Creek
16) Honeoye Creek
17) Spring Brook
18) Mill Creek (Honeoye Park)
19) Bradner Creek
20) Stony Brook
21) Sugar Creek
22) Ewart Creek
23) Cold Creek
24) Rush Creek
25) Crawford Creek
26) Wigwam Creek
27) White Creek (Belfast)
28) Baker Creek
29) Black Creek (Benetts)
30) Phillips Creek
31) Knight Creek
32) Vandermark Creek
33) Brimmer Brook
34) Elm Valley Creek
35) Railroad Brook
36) East Valley Creek
37) Dyke Creek
38) Quig Hollow Brook
39) Ford Creek
40) Marsh Creek
41) Chenunda Creek
42) Cryder Creek

Streams sampled after Hurricane Agnes

43) Genesee River (Rochester)
44) Genesee River (Avon)
45) Genesee River (Mount Morris)
46) Canaseraga Creek (Dansville)
47) Genesee River (Portageville)
48) Genesee River (Wellsville)

TABLE 1

DESCRIPTION OF LAND USE, SOILS DATA AND BEDROCK GEOLOGY FOR THE SEVEN PRE-STORM Q-MODE CLUSTERS

Q-mode Cluster	Number of Watersheds	Dominant Land Use	Soils Data			Bedrock Geology
			Texture	pH	Drainage	
A_1	6	Forest - 6	Slightly coarse	Acidic	Somewhat poor	Upper Devonian shale and siltstone
A_2	5	Forest - 4 Agriculture) - 1 and forest)	Coarse	Acidic	Moderate	Upper Devonian shale and siltstone with some sandstone
A_3	3	Forest - 3	Slightly coarse	Slightly acidic	Somewhat poor	Upper Devonian shale and siltstone
A_4	5	Forest - 5	Slightly coarse	Acidic	Moderate	Upper Devonian shale and siltstone
B	4	Agriculture - 2 Agriculture) with some)- 2 forest)	Slightly coarse	Acidic	No trend	Upper Devonian shale and sandstone with some siltstone
E	8	Agriculture - 8	Fine	Basic	Well-drained	Middle Devonian shale and limestone with some upper Devonian shale and limestone
F	4	Agriculture - 4	No trend	Slightly basic	Well-drained	Upper Silurian shale, dolostone, salt and gypsum

TABLE 2

AVERAGE CHEMISTRY

Q-mode Cluster	Number of Watersheds	Chloride (mg/l)		Nitrate-Nitrogen (mg/l)		Alkalinity (mg/l)	
		Avg	Range	Avg	Range	Avg	Range
A_1	6	21.1	1.9-81	0.03	.01-.07	64	54-80
A_2	5	9.9	3-26	0.16	.01-.30	58	34-74
A_3	3	3.4	2.2-5	0.01	.01-.20	93	83-99
A_4	5	4.8	1.7-9.8	0.18	.04-.30	26	16-32
B	4	11.7	5.7-20	1.23	.07-1.80	119	97-128
E	8	44.5	27-72	0.84	.02-2.70	204	128-245
F	4	48.8	36-69	0.98	.70-1.30	234	194-291

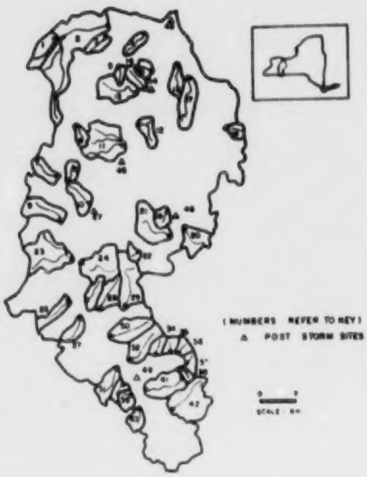

(NUMBERS REFER TO KEY)
△ POST STORM SITES

Figure 1. Location of Sub-Watersheds Sampled During June, 1972

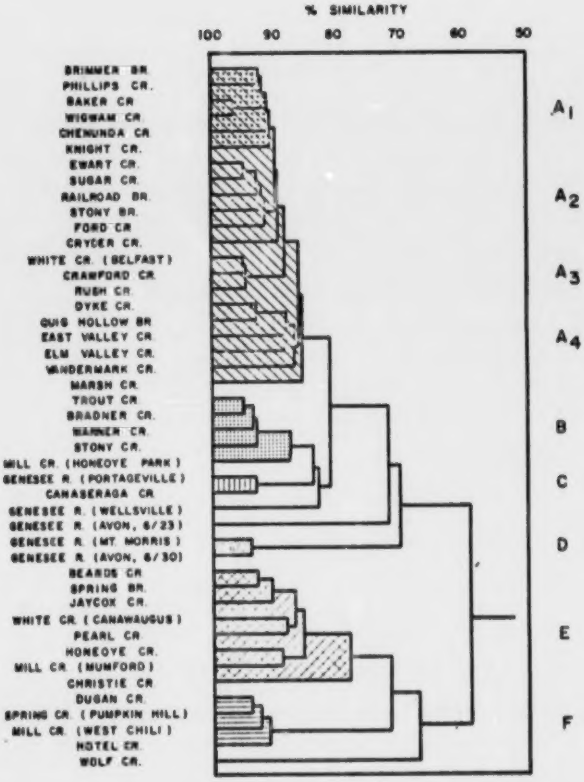


FIGURE 2. Q-MODE DENDROGRAM OF GENESEE DATA.

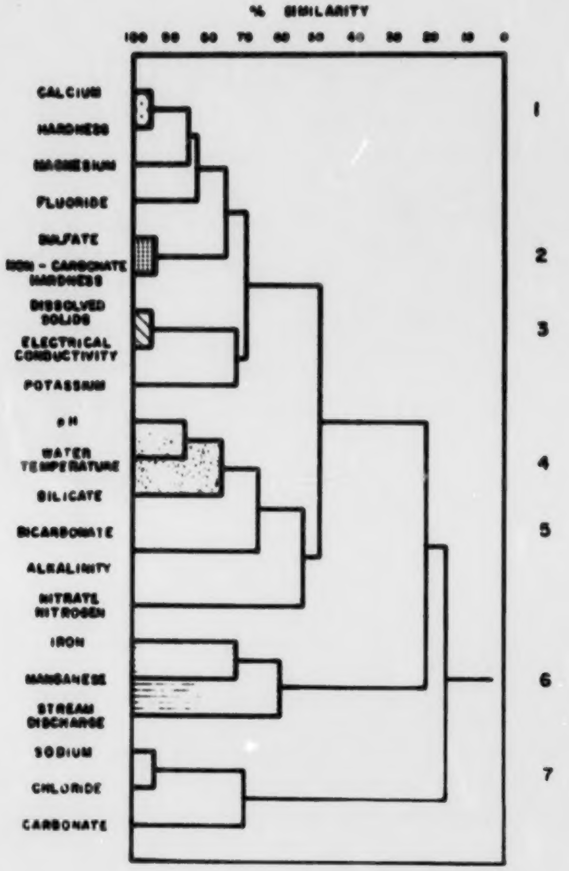


FIGURE 3. R-MODE DENDROGRAM OF GENESEE DATA.

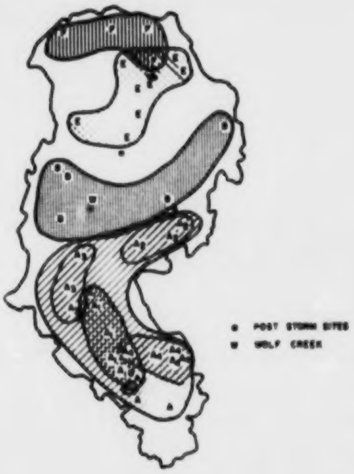

● POST STORM SITES
■ WOLF CREEK

Figure 4. Geographic Distribution of Q-Mode Clusters

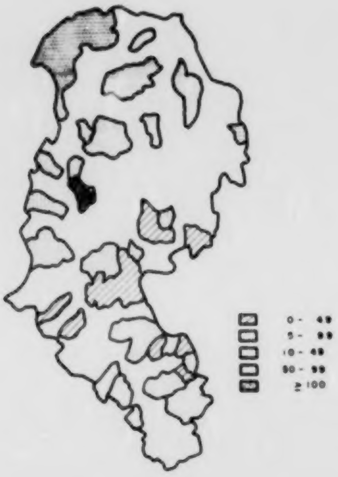

0 - 49
5 - 99
10 - 49
50 - 99
≥ 100

Figure 5. Geographic Distribution of Chloride (mg/l)

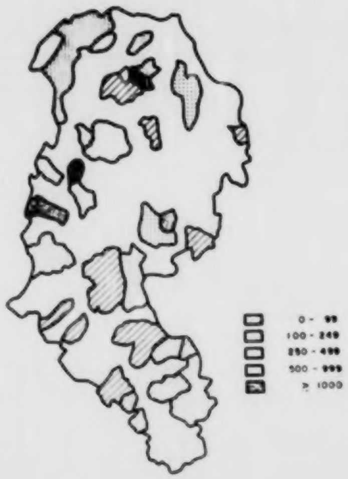

0 - 99
100 - 249
250 - 499
500 - 999
≥ 1000

Figure 6. Geographic Distribution of Disolved NO_3-N (μg/l)

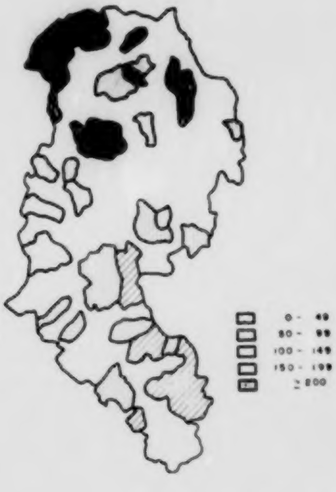

0 - 49
50 - 99
100 - 149
150 - 199
≥ 200

Figure 7. Geographic Distribution of Alkalinity (mg/l)

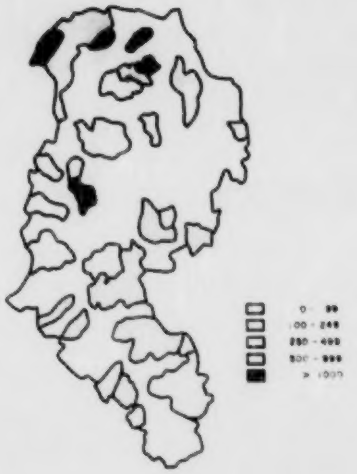

0 - 99
100 - 249
250 - 499
500 - 999
≥ 1000

Figure 8. Geographic Distribution of Electrical Conductivity (μ mhos/cm)

FIGURE 9. Q-MODE DENDROGRAM OF MILL CREEK DATA

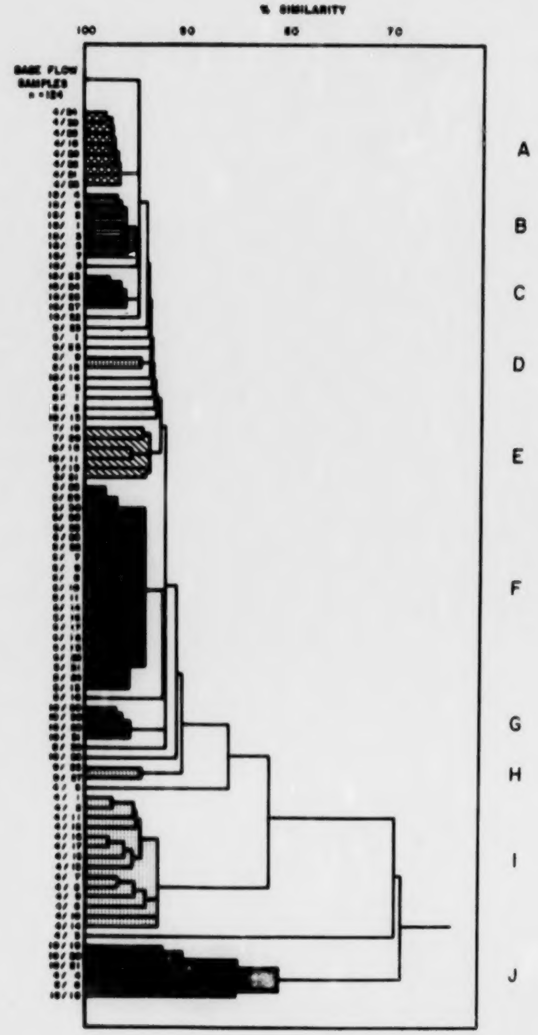
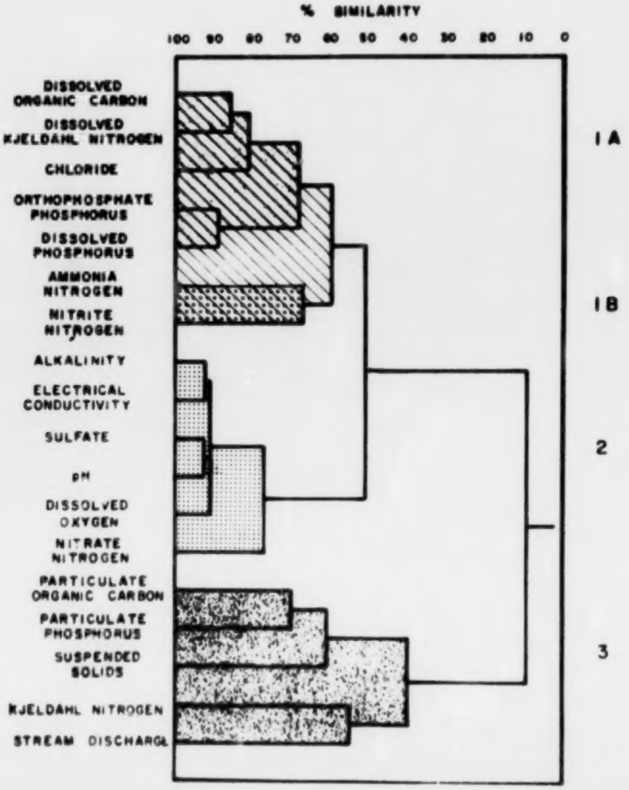


FIGURE 10. R-MODE DENDROGRAM OF MILL CREEK DATA



APPLICATION OF PATH ANALYSIS TO DELINEATE THE SECONDARY GROWTH EFFECTS OF MAJOR LAND USE PROJECTS

Tom McCurdy, Environmental Planner
Strategies and Air Standards Division, EPA, Durham, North Carolina

Frank Benesh, Environmental Planner Peter Guldberg, Senior Scientist
Walden Research, Cambridge, Massachusetts

Dr. Ralph D'Agostino
Professor of Mathematics, Boston University

Abstract

This paper presents a path analytic modeling process used to test various factor theories of induced urban development. The original and final "trimmed" path models are discussed, as well as statistical problems associated with using path analysis to describe a non-recursive system.

Introduction

This path analysis effort is a part of an Environmental Protection Agency (EPA) project entitled "Growth Effects of Major Land Use Projects", or GEMLUP for short.

The main purpose of GEMLUP is to formulate a non-proprietary statistical methodology to predict air pollution emissions from (1) two major land use development types--large places of employment and large residential projects,* (2) secondary development that is induced** by the major project, and (3) motor vehicular traffic associated with both kinds of urban development. Subsidiary purposes are to formulate and test a factory theory of induced development using path analysis and to generate and apply land use oriented emission factors based on current energy consumption data.[1]

GEMLUP relates to a number of EPA programs, including air quality maintenance areas (AQMA) planning[2], environmental impact statement (EIS) review[3], the indefinitely suspended portions of indirect source review[4], and the prevention of significant air quality deterioration, or non-degradation.[5] Explicit or implicit in these programs is an evaluation of air quality impacts of land use plans or project developments, but the Agency does not provide, specify, or recommend a method for evaluation in any of the programs. GEMLUP is designed to formulate and test a method of evaluating land use impacts at the project level.

Theory and Approach

Of the many types of scientific theory discussed in the literature***, the most rigorous type of theory that we could ascribe to is "factor theory," which is characterized by narrow and non-overlapping generalizations, a selective, explicit enumeration of (all) factors thought to influence a given phenomenon, and the utilization of empirically defined variables to represent the factors involved. While almost every effort at causal explanation involves factor theory, it is limited theory because it does not readily suggest other generalizations, due to its relatively narrow focus[6]. Consequently, we had to operationalize the factor theory by using a model. The next step was then clear: formulate a theory of induced development and choose a model to test it.

A Theory of Induced Development

Taking the industrial/offices major land use project type as the more general case of the two types investigated, we devised the following theory of induced development.*

Constructing a large source of employment like an industrial/office complex generates jobs which result in the nearby construction of dwelling units; these induce retail development to locate near them and generate demand for community, cultural, and religious facilities (schools, recreation areas, libraries, churches, theaters, fire and police stations, etc.). All of this requires the construction of streets and highways that then improve accessibility to the area. Better access fosters continued urban development, particularly highway-oriented commercial and office land uses. Additional sources of employment come into the area as secondary (and tertiary) industry or services located near the original major project, spurring on another round of residential development, and so forth. This can be summarized as:

$$\text{induced land use} = f\,(\text{size of major project, other endogenous variables, other exogenous variables}) \quad (1)$$

where the other endogenous variables are the other induced land uses in the model and the other exogenous variables are vacancy rates, accessibility measures, etc. which affect the influence of the major project on induced development.

That is what was hypothesized to happen. As can be noted, feedback in the system was explicitly hypothesized. Our theory also specified that within a 10,000 acre circular "area of influence" centered on the original major land use project, all of the above development would occur within ten years after the employment source opened. Our rationale for the where and when will have to be discussed elsewhere.[11] The structural equations and path analytic diagrams discussed below rigorously depict the model used to test the theory; however, we still must explain why we chose path analysis as the modeling methodology in the first place.

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*Definitions of the project types investigated in GEMLUP are:

1. Place of employment: an office building or complex, an industrial building or complex, or a research and development building or complex constructed between 1954 and 1964 and having a minimum employment of 2,250 persons within five years of initial operation.

2. Residential project: an apartment structure or complex, residential subdivision, planned unit development, or new town constructed between 1954 and 1964 and having a minimum population of 4,500 persons within five years of initial occupancy.

**Induced development is land use development caused by, or constructed because of, the major land use project.

***See references 6-10.

*The theory is not entirely new. Most of the urban development models referenced in the next section are based upon the same general relationships posited in our theory, though they are usually less explicit than ours.

Analytic Approach

Part of the reason for using path analysis to test our theory was programmatic: we did not have time or money to do more. For instance, the highly detailed deterministic approaches patterned after Lowry[12] or Forrester[13] or others working in the same vein* were simply infeasible. They were also inappropriate because of their concern with highly aggregated regional development and/or long planning horizons. Because of this and the problems associated with deterministically modeling a social system, it was decided to utilize a statistical or probabilistic approach.

It was also obvious that a dynamic modeling approach was infeasible because of the effort involved in obtaining longitudinal data to incorporate time into the system and in solving the simultaneous differential equations involved. For similar reasons, a difference equation approach (i.e. predicting the change in land use over the ten year period) was also infeasible. The static approach to testing our inherently change-oriented theory is justified by three factors: (1) our theoretical assumption that induced development follows a *single* basis causal structure for all cases or observations, (2) the use of a cross-sectional method of obtaining data for variables observed in a static state and the assumption that input variables were initialized at time 0 and held constant long enough so that all the causal consequences in the system were realized, and (3) the use of certain time-lagged exogenous variables in the system. The conceptual usefulness of these factors in testing causal theory is well described in Heise[19] and Blalock.[20]

Conceptually, the total land use in the 10,000 acre area of influence at the end of the ten year time period can be defined as three components:

$$\begin{aligned}&\text{total land use}_{t+10} = \\ &(\text{prior land use}_t)+(\text{project induced land use}_{t\to t+10})+(\text{non project induced land use}_{t\to t+10}) \qquad (2)\end{aligned}$$

The prior land use in time t is the amount of land use existing in the year of the initial occupancy of the major project. Non project induced land use in the period t to t+10 is the amount of land use growth, t to t+10, that occurred in the area of influence but was not induced by the major project. The non project induced land use includes growth due to regional expansion and random effects.

The selection of a cross sectional approach limited our model to the prediction of the total land use in the year t+10. Consequently, the basic structure of our model is a series of simultaneous equations of the following form:

$$\text{total land use}_{t+10} = f(\text{Type I variables, Type II variables}) \qquad (3)$$

where Type I variables are predictors of the induced portion of the total land use (see Equation 1) and Type II variables are predictors of the prior land use in year t and non project induced land use in the period t to t+10.

Finally, there was not enough existing information on project-level induced development to be able to define the form of the relationships in the system. The form, therefore, was assumed to be linear. This is not a bad *a priori* approximation in most social science applications, and it allows the use of well developed statistical techniques. There is accumulating evidence that many social systems can be approximated by a linear function as long as operating conditions remain fairly stable.[19] Even complex non-linear relationships can often be approximated by a constant relation in discrete subregions of the relationship.[21] Also, if a relationship is thought to be nonlinear on theoretical grounds (e.g., multiplicative, exponential), the data can be transformed prior to entering it in the linear analysis.[22]

For all of these reasons, the path analytic technique based on multiple regression analysis seemed appropriate to test our theory of induced development. Path analysis was developed by biologist Sewall Wright in the 1920's as a technique for examining observed interrelated variables that are assumed to be completely determined by exogenous variables.

> It is not capable of deducing causal relations from available quantitative information (viz., correlation coefficients), but rather it is intended to combine this quantitative information with qualitative information that is available on the causal relations to give a quantitative interpretation. It is a technique useful in testing theories rather than in generating them and it can be used to study the logical consequences of various hypotheses involving causal relations. In order to implement the technique, the researcher must make explicit a theoretical framework or model.[22]

Use of the technique requires two assumptions about causality in the system: (1) a *weak* causal order exists among the variables and it is *known*, and (2) relationships among variables are causally closed. Weak causal ordering exists in a two variable set, X_i and X_j, it it is known on logical, empirical, or theoretical grounds that X_i *may* (or may not) affect X_j and that X_j *cannot* affect X_i. Causal closure is simply the concept that given a bivariant covariation between X_i and X_j and weak causal ordering ($X_i \rightarrow X_j$), the observed covariation between the two variables must be due to the causal dependence of X_j on X_i, their mutual dependence on some outside variable(s), or a combination of these two factors.[23]

Path diagrams (see below) depict the hypothesized causal relations among variables. Causality is shown by a single-headed arrow (or path) and interaction (correlation) between two variables is shown by a curving double headed arrow. A coefficient P_{ij} is associated with each path and can be interpreted as a regression coefficient; that is, the amount of change in the dependent variable caused by a one unit change in the independent variable with all other independent variables held constant. The coefficient on the interaction arrows is the correlation coefficient R_{ij}. All of the statistical assumptions of regression analysis (e.g., independence of observations, uncorrelated residuals, a normal distribution of means of sample data) apply to path analysis as well.

Path analysis has been used at least once before in environmental modeling. Researchers at Argonne National Laboratories chose the technique to causally relate four independent variables (land area, number of employees, process weight rate, and energy use) to a dependent variable, regulated point source emissions of particulate air pollution.[24] While the authors were unhappy because land area and number of employees did not relate well to the dependent variable, the relationships depicted in the system are logical and certain of the path coefficients are significant.

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*Hill [14], Seidman [15], and Center for Real Estate and Urban Economics [16]. In addition to these general or comprehensive models, there are many single sector models that have been developed since the early 1960's. See references 17 and 18 for a review of urban development models.

Model Specification

The theory of induced development was translated into two models, a residential project model and an industrial/office project model. Due to the limited length of this paper, only the industrial/office model will be discussed. The specification and testing of the residential model was undertaken in a similar manner.

The industrial/office project model was specified as 13 equations, 5 of which are simultaneous and the remaining 7 are recursive. The path diagram of the model is shown in Figure 1. The definition of each variable is shown in Table 1. The theoretical basis of each path is discussed elsewhere.[25]

Methodological Issues

Based on certain criteria, the most important criterion being the minimum size of major project (see page 1), a sample of twenty case studies of each major project type was selected. The size of the sample was limited by available resources (over 7½ man-months was required to collect data for the present sample). This small sample size created two important methodological problems.

Degrees of Freedom in First Stage of Two Stage Least Squares

While one would prefer as large a sample as possible, the use of a sample of twenty in an ordinary least squares regression with four or five independent variables, such as in the seven recursive equations of our model, is not uncommon. However, in the specification of our model there is a simultaneous block of five equations. In this situation it would be inappropriate to use ordinary least squares (OLSQ), as such a technique would produce biased and inconsistent estimates. Accordingly, we made use of the two stage least squares (2SLS) technique to estimate the structural coefficients in the five simultaneous equations. As the first stage of 2SLS estimates the right hand side endogenous variables with all the exogenous variables in the simultaneous block, the degrees of freedom in the first stage of the 2SLS in our analysis is zero. (There are twenty exogenous variables).

Our approach to solving this problem was to use stepwise OLSQ to delete those instrumental variables that were insignificant in the first stage of the 2SLS. First, one instrumental variable for each endogenous variable was identified as having the strongest *a priori* causal influence. These five variables, in addition to the major project size, were entered in the first step of a stepwise OLSQ predicting each endogenous variable. (This was done to insure identification). Then the others were allowed to enter in the order of their significance of their added partial contributions. The seven instrumentals that overall were of least significance were deleted. This left 6 degrees of freedom (20-1-13=6) for the first stage of the 2SLS.

Stability of Estimated Coefficients

In order for path analysis to be of use the resulting estimates should be stable. They will be of little use if they change radically depending on sample observations. In most applications of path analysis, this is achieved by using large samples and reliable measuring instruments. In our application, with a sample of twenty, the stability of the estimates must be explicitly addressed.

Our approach to this problem involved the use of the statistical techniques of "Jack-Knife". Instead of running one regression using twenty observations, 20

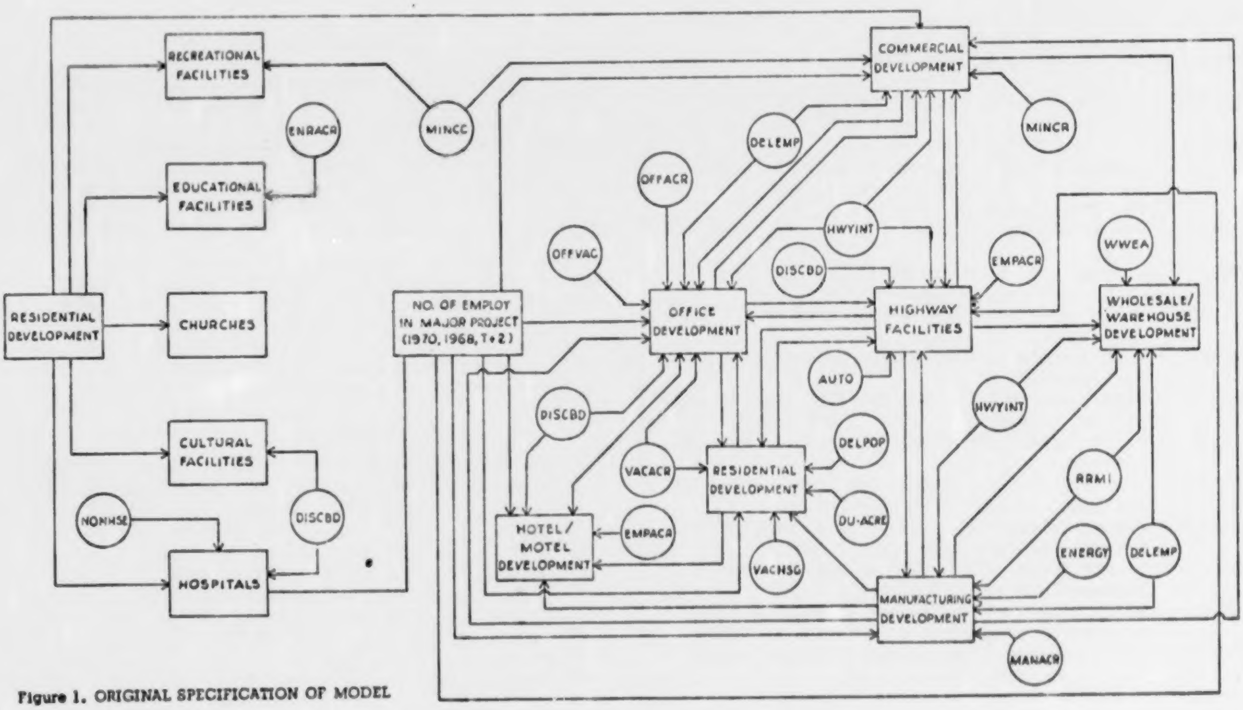
COMMERCIAL DEVELOPMENT
RECREATIONAL FACILITIES
MINCC
MINCR
ENRACR
DELEMP
OFFACR
EDUCATIONAL FACILITIES
HWYINT
WWEA
OFFVAC
DISCBD
EMPACR
RESIDENTIAL DEVELOPMENT
CHURCHES
NO. OF EMPLOY IN MAJOR PROJECT (1970, 1968, T+2)
OFFICE DEVELOPMENT
HIGHWAY FACILITIES
WHOLESALE/ WAREHOUSE DEVELOPMENT
AUTO
DISCBD
HWYINT
DELPOP
CULTURAL FACILITIES
VACACR
RESIDENTIAL DEVELOPMENT
RRMI
NONHSE
DISCBD
DU-ACRE
HOTEL/ MOTEL DEVELOPMENT
EMPACR
ENERGY
DELEMP
HOSPITALS
VACHSG
MANUFACTURING DEVELOPMENT
MANACR

Figure 1. ORIGINAL SPECIFICATION OF MODEL

Table 1
MODEL VARIABLES AND DEFINITIONS

RES = number of housing units in area of influence in 1970 (excluding major project).
COMM = commercial land use in area of influence in 1970 in 1,000 square feet.
OFFICE = office land use in area of influence (excluding major project) in 1970 in 1,000 sq. feet.
MANF = manufacturing land use in area of influence (excluding major project) in 1970 in 1,000 square feet.
WHOLE = wholesale/warehouse land use in area of influence in 1970 in 1,000 square feet.
HOTEL = Hotel and motel land use in area of influence in 1970 in 1,000 square feet.
HOSPTL = hospital, etc. land use in area of influence in 1970 in 1,000 square feet.
CULTUR = cultural land use in area of influence in 1970 in 1,000 square feet.
CHURCH = religious land use in area of influence in 1970 in 1,000 square feet.
ED = public educational land use in area of influence in 1970 in 1,000 square feet.
REC = active outdoor recreational land use in area of influence.
HWLM - highway lane miles in area of influence in 1970.
DU-ACRE = dwelling units per acre in area of influence in 1960.
VACACR = percent vacant developable acreage in area of influence in year (t + 0)
VACHSG = percent vacant housing in area of influence in 1960.
HWYINT = highway interchanges in area of influence in year (t + 5)
MINCC = median income of families and individuals in area of influence relative to U.S. median income in 1960.
INCMP = variable indicating the median income level of major project compared to surrounding community in year (t + 2)
OFFVAC = percent office buildings vacant in metropolitan area in year (t + 0)
OFFACR = office employment per acre in area of influence in year (t + 0)
DISCBD = distance from center of major project to CBD in year (t + 0)
ENERGY = cost factor for electricity ($/1500 KWH) for commercial users in the metropolitan area in year (t + 0) divided by the average U.S. commercial rate in 1960.
RRMI = railroad mileage in area of influence in year (t + 0)
WWEA = warehouse and wholesale employment per acre in area of influence in year (t + 0)
EMPACR = total employment per acre in area of influence in year (t + 0)
NONHSE = nonhousehold population per acre in area of influence in 1960.
MPKIDS = school-age children per dwelling unit in major project in year (t + 2)
ENRACR = public school enrollment per acre in area of influence in 1960.
MANACR = manufacturing employment per acre in area of influence in year (t + 0)
DELPOP = growth factor for total regional population between 1960 and 1970 (county data)
DELEMP = growth factor for total regional employment between 1960 and 1970 (county data)
MINCR = median income of the region in year (t + 0) relative to the median U.S. income in 1960.
MAJOR PROJECT = number of employees in major project in 1970, 1968, t + 2.
AUTO = automobile drivers per acre in country in 1960.

regressions are run each containing nineteen observations. The path coefficients are then examined for stability. In our analysis, after trimming the model to a final set of path coefficients, each equation was subjected to a jack-knife. The brevity of this paper does not permit the presentation of this analysis. It is discussed elsewhere.[25]

Path Analysis of Model

Our approach to path analysis was to develop the most elaborate system possible, given the sample size, and then after estimating the involved path coefficients, refine or trim the system by dropping those paths that have coefficients that are "close to zero". The original model was thus refined or trimmed and thereby made more parsimonious.

Specifically, we retained a specific path if
- its t value exceeded unity in absolute value. This guaranteed that the adjusted R^2 is larger with its inclusion that without its inclusion for OLSQ.)
- its beta weight exceeded .1 in absolute value. This was judged to reflect a substantially meaningful relation, and
- it was deemed a priori to be of substantive importance and its sign (i.e., the sign of the coefficient b) was of the expected direction.

It is important to note that our trimming procedure was an interactive process; at each step the remaining path coefficients were examined to see how the deletion of one path coefficient affected our ability to reproduce the original observed correlations. This is particularly critical in 2SLS, where the deletion of one exogenous variable in one equation can effect another equation because of its deletion as an instrumental variable.

Following the above procedure, the original path diagram was trimmed to model shown in Figure 2. The number on each path is the path coefficient; the number inside the box of an endogenous variable is the R^2 of the equation predicting that variable.

Summary of Results

In general, the trimmed path model is a successful test of our theory of induced developments. The size of the major project in time t+10 was specified as an exogenous variable in the residential, commercial, office, manufacturing, highway facilities, hotel/motel, and hospital equations. Though it was trimmed from the hospital and highway facilities equations, its causal influence in the remaining equations was substantial.

Additionally, the causal analysis of the model leads us to be optomistic about the model's subsequent calibration. Pending the calibration and a possible validation study, our preliminary assessment is that the static cross-sectional modeling approach can be used to predict the induced land uses from the construction and operation of a major land use development.

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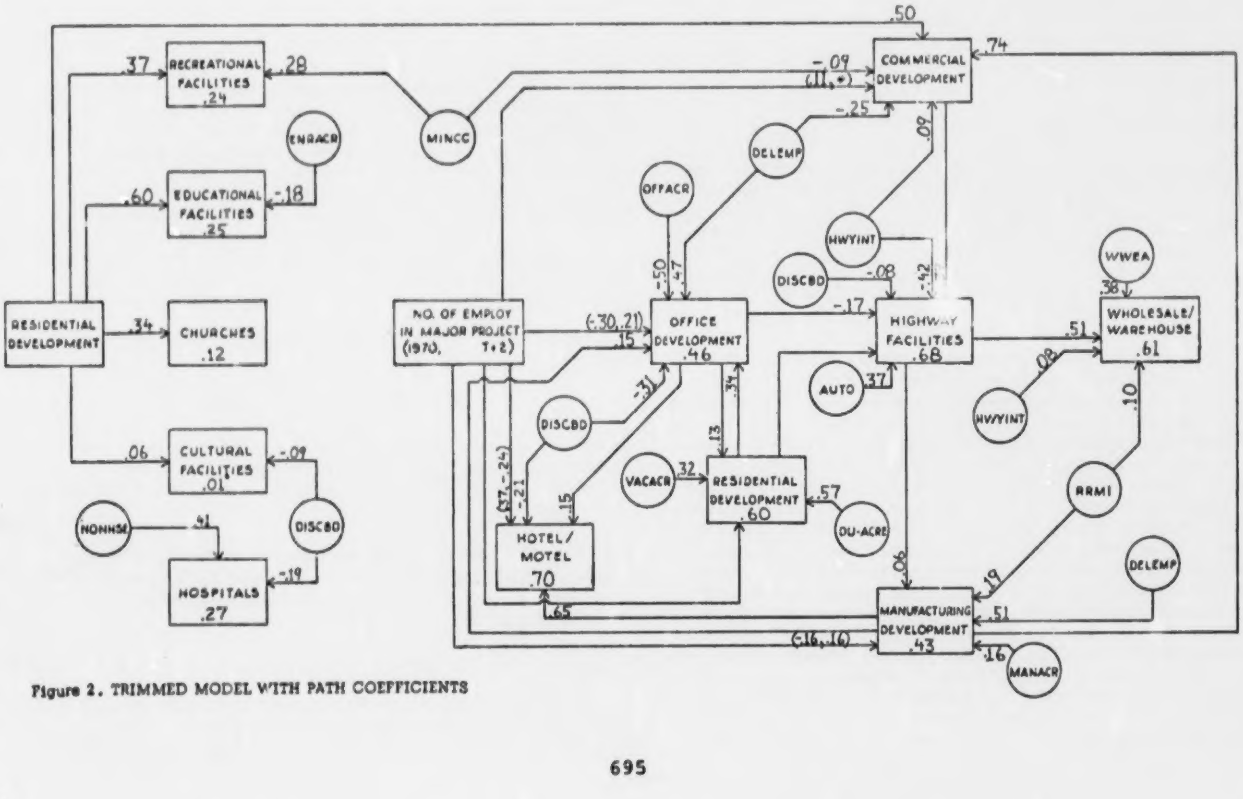
RESIDENTIAL DEVELOPMENT
.37
RECREATIONAL FACILITIES .24
.28
MINCC
ENRACR
.60
EDUCATIONAL FACILITIES .25
-.18
.34
CHURCHES .12
.06
CULTURAL FACILITIES .01
-.09
DISCBD
NONHSE
.41
HOSPITALS .27
-.19
NO. OF EMPLOY IN MAJOR PROJECT (1970, T+2)
(-.30,.21)
.15
OFFICE DEVELOPMENT .46
OFFACR
-.50
.47
DELEMP
-.25
.50
-.09
(.11,*)
COMMERCIAL DEVELOPMENT
.74
.09
HWYINT
DISCBD
-.08
-.42
-.17
HIGHWAY FACILITIES .68
AUTO
.37
.51
WWEA
.38
WHOLESALE/ WAREHOUSE .61
HWYINT
.08
.10
RRMI
.19
DISCBD
-.31
(.37,-.24)
-.21
.15
HOTEL/ MOTEL .70
.65
.34
.13
VACACR
.32
RESIDENTIAL DEVELOPMENT .60
.57
DU-ACRE
.06
MANUFACTURING DEVELOPMENT .43
DELEMP
.51
(-.16,.16)
.16
MANACR

Figure 2. TRIMMED MODEL WITH PATH COEFFICIENTS

PREDICTION OF PHYTOPLANKTON PRODUCTIVITY IN LAKES

V. W. Lambou, L. R. Williams, S. C. Hern, R. W. Thomas, J. D. Bliss
Water and Land Quality Branch, Monitoring Operations Division
Environmental Monitoring and Support Laboratory
U.S. Environmental Protection Agency
Las Vegas, Nevada

SUMMARY

This study presents relationships between phytoplankton productivity as measured by yearly mean chlorophyll *a* levels, and ambient water quality and hydrologic measurements. Among the nutrients examined, phosphorus forms were most highly correlated with chlorophyll *a* levels. The effects of such factors as retention time, primary nutrient limitation, stratification, and macrophyte dominance upon productivity responses are evaluated. Additional parameters related to productivity include turbidity, Secchi disc, nitrogen to phosphorus ratio, pH, total alkalinity, and forms of inorganic nitrogen. Discussions of the factors affecting phytoplankton productivity and the application of the limiting nutrient concept are included.

INTRODUCTION

The National Eutrophication Survey was initiated in 1972 in response to an Administration commitment to investigate the nationwide threat of accelerated eutrophication to freshwater lakes and reservoirs. Consistent with the Survey objectives to develop information on nutrient sources and impact on freshwater lakes, we are examining relationships between ambient nutrient concentrations and existing lake conditions.

The purpose of this report is to help to establish lake classes and elucidate the relationships between ambient nutrients and lake water quality by lake type. The data were collected in 1972 from the New England States, New York, Michigan, Wisconsin, and Minnesota. Only lakes sampled during three seasonal sampling rounds are included.

MATERIALS AND METHODS

Lake Selection: Selection of lakes and reservoirs included in the Survey in 1972 was limited to lakes 40 hectares or more in surface area, with mean hydraulic retention times of at least 30 days, and impacted by municipal sewage treatment plant (MSTP) effluent either directly or by discharge to an inlet tributary within 40 kilometers (km) of the lake. Specific selection criteria were waived for lakes of special State interest.

Lake Sampling: Sampling was accomplished by two teams, each consisting of a limnologist, pilot, and sampling technician, operating from pontoon-equipped helicopters. With few exceptions, each lake was sampled under spring, summer, and fall conditions. Sampling site locations were chosen to define the character of the lake water as a whole and to investigate visible or known problem areas, e.g., algal blooms, sediment or effluent plumes. The number of sites was limited by the survey nature of the program and varied in accordance with lake size, morphological and hydrological complexity, and practical considerations of time, flight range, and weather. At each sampling depth, water samples were collected for nutrient, alkalinity, pH, conductivity, and dissolved oxygen determinations. Contact sensor packages were used to measure depth, conductivity, turbidity, pH, dissolved oxygen, and temperature. Fluorometric chlorophyll *a* (chl*a*) analyses were performed at the end of each day in the mobile laboratory. Nutrients and alkalinity were determined by automated adaptations of procedures described in "Methods for Chemical Analysis of Water and Wastes"[1] at the Las Vegas laboratory. Details of Survey methods are presented elsewhere.[2,3]

Data Management: Data collected were stored in STORET and manipulated, as prescribed by Bliss, Friedland, and Hodsen.[4] Basic calculations for parameters measured in sampled lakes were performed in such a way to give equal weight to: each depth sampled at a station; each sampling station sampled on an individual lake during a sampling round; and each sampling round on an individual lake during a sampling year.

Mean parameter values for each sampling station were calculated as follows:

$$\overline{Par_j} = \sum_{i=1}^{D} Par_i/D, \tag{1}$$

where $\overline{Par_j}$ = mean value for a parameter at the j^{th} sampling station during a sampling round, Par_i = value for the i^{th} depth, and D = the number of depths for which a parameter was measured at the j^{th} sampling station during a sampling round. Mean parameter values for each sampling round were calculated as follows:

$$\overline{\overline{Par_k}} = \sum_{j=1}^{S} \overline{Par_j}/S, \tag{2}$$

where $\overline{\overline{Par_k}}$ = mean value for the k^{th} sampling round on a given lake, and S = number of sampling sites. Mean lake parameter values for a given sampling year were calculated as follows:

$$\overline{\overline{\overline{Par}}} = \sum_{k=1}^{3} \overline{\overline{Par_k}}/3, \tag{3}$$

where Par = mean parameter value for a given sampling year. Lake parameter values were calculated only when values were available for the first, second, and third sampling rounds during a given sampling year from a lake. Formulas 1, 2, and 3 were used to determine parameter values for total phosphorus (TP), dissolved phosphorus (DP), ammonia-N (NH), nitrite-nitrate-N (NO), ammonia-nitrite-nitrate-N (IN), and total alkalinity (AL), all expressed in milligrams per liter (mg/liter), temperature in degrees Celsius (°C)(T), turbidity in percent transmission (TB), pH (PH), Secchi disc in inches (SD), and hydraulic retention time in days (RT).

The ratio of IN/DP (N/P) for each sampling station was calculated as follows:

$$\overline{N/P} = \overline{IN}/\overline{DP}, \tag{4}$$

however, at the formula 1 level a dissolved phosphorus value was deleted if either nitrogen complement was missing. Round and yearly values were calculated using formulas 2 and 3.

Unlike the above parameters where measurements were made at various depths, only one chl*a* measurement was made at any individual sampling station during a sampling round. Therefore,

$$\overline{chla_j} = chla \tag{5}$$

where $chla_j$ = the mean chl*a* concentration in micrograms per liter (µg/liter) for the j^{th} sampling station during a sampling round, and chl*a* = the chl*a* concentration in μg/liter for an integrated water sample from the surface to 4.6 meters (m) or to a point just off the bottom when the depth was less than 4.6 m.

DATA LIMITATIONS

The primary selection criterion for the 1972 Survey lakes was direct or indirect receipt of MSTP effluent (151 out of 191 lakes), resulting in a list of obvious bias. Fortunately, special interest lakes, representing a broad range of water quality, were also included which provided some trophic balance to the list. Although lakes selected were not necessarily representative of average conditions existing in the study area, the relationships observed between ambient nutrients and lake water quality should not be biased.

A number of factors required for a complete nutrient budget analysis have not been evaluated thus far. Among these factors are the following: 1) groundwater contributions were not considered; 2) macrophytes were not measured quantitatively; 3) nitrogen-fixation was not estimated; 4) coincidence of sampling with "turnover" or macrophyte nutrient release periods was not sufficiently precise to make accurate estimates of nutrient maxima; 5) no estimates of sediment load, sediment-water nutrient exchange or sediment binding capacity were made; and 6) sampling frequency was generally inadequate to determine dynamic changes in nutrient limitation, where present; however, seasonal shifts could be determined.

LIMITING NUTRIENTS

Nitrogen and phosphorus are frequently mentioned as the nutrients most likely to limit growth of plants. The concept of a limiting nutrient, as related to Leibig's Law of the Minimum, is that some nutrient, least available relative to the growth requirements of a given organism, imposes primary limitation on the growth of that organism.

The Algal Assay Procedure Bottle Test[5] utilizes the response of the green alga *Selenastrum capricornutum* to nutrient spikes, usually nitrogen and phosphorus, alone and in concert, to determine the growth-limiting nutrient. The assumption is that if indeed a specific nutrient is limiting the growth of the algal culture, addition of that nutrient will result in a positive growth response. If the addition of the "limiting nutrient" is large enough, growth will proceed until another takes over the controlling role, now being the least available relative to the growth needs of the culture. Various estimates have been proposed as to what constitutes that ratio of nitrogen to phosphorus at which the addition of either results in the limitation by the other. Such estimates have been reported as low as 5/1 and as high as 30/1 or more, by weight, generally centering about 12/1 to 14/1. These are in reasonable agreement with theoretical needs based upon stoichiometric equations of algal constituents.[6]

Frequency distributions of the ratios of inorganic to orthophosphorus (N/OP) were determined from chemistries taken on fall samples just prior to algal assay.[2,3] Among the nitrogen-limited (N-limited) lakes (by algal assay) the N/OP values were distributed as follows: <10 = 60 lakes; 10 to 14 = 10; and >14 = 1. For the phosphorus-limited (P-limited) lake group the values were: <10 = 3 lakes; 10 to 14 = 7; and >14 = 59. Note the overlap of P- and N-limited lakes in the zone extending from N/OP = 9 to 15. Within this range fell several additional lakes which evidenced "co-limitation" on assay and were included in neither distribution. In these samples no growth response was noted with the addition of *either* nitrogen or phosphorus, but response was dramatic to the simultaneous addition of both.

We divided the lakes sampled into P-limited ($N/P>14$), transition ($10<N/P>14$), and N-limited ($N/P<10$) groups based upon the yearly mean N/P observed in the lake. The frequency distribution of N/P values was: <10 = 79 lakes; 10 to 14 = 44; and >14 = 69. While admittedly arbitrary, the suggested division represents a convenient means of comparing groups of lakes presumably representing "largely nitrogen-limited" and "largely phosphorus-limited" populations, and a third group, representing a buffer between the first two groups. This group contains a number of lakes whose N/P ratios, by sampling round, suggest seasonal shifts from one dominant limiting nutrient to the other across a transition zone in which pronounced interaction is likely.

The ranges selected are not suggested to possess sharp cutoffs at which shifts in limiting nutrient occur. Preliminary analyses of Survey algal assay data suggest that any such sharp cutoff is unlikely with laboratory monocultures, much less with mixed natural populations. Rather the N- and P-limited groups represent "tails" toward which the influence of the secondary interactant is progressively reduced. Also, as N/P ratios progressively deviate from the buffer zone in either direction, the influence of the secondary interactant is continually reduced. Chiaudani and Vighi[7] present data which suggest a range of N/P ratios about four to five units wide within which neither nitrogen nor phosphorus effects are independent. However, they found no response to phosphorus addition below N/P = 10 with *Selenastrum*.

While the limiting nutrient concept has some utility in allowing prediction of the potential growth limits of laboratory monocultures, its extrapolation into natural system studies should be approached warily. A number of enrichment studies have found the effects of phosphorus and nitrogen to be interdependent,[8,9,10,11] modified by the presence of trace organic materials in the waters,[12] and dependent upon previous algal culture exposure, i.e., prior luxury uptake of nitrogen or phosphorus.

It is not unlikely that a mixed natural phytoplankton population would contain elements with a range of optimal growth requirements and predisposing nutritional status. Addition of either nitrogen or phosphorus could potentially evoke a net increase in phytoplankton growth, especially in those cases in which the ambient N/P ratio is intermediate between the optimal growth requirements of the various phytoplankton elements. The presence of organic materials may increase nutrient assimilation in some members of the community[9,12] or inhibit it in others.[13] Conditions may exist, over a range of N/P values, favoring response to the addition of either phosphorus or nitrogen and representing essentially "net co-limitation." Different species within a community may be limited by different nutrients simultaneously.[14] A theoretical basis for simultaneous co-regulation of the specific growth rate of a single population by multiple nutrient is presented by Sykes.[15] Verduin[16] proposes the use of the Baule-Mitscherlich equation, with slight modification, to predict yield as a product of the levels of interacting nutrients. The goodness-of-fit of the "Verduin model" is presently being tested with the Survey data base; the results will be reported in the near future.

Although phosphorus and nitrogen are considered the most important limiting nutrients in freshwaters[6] and the supply of inorganic carbon and total carbonate is in excess in most natural waters[1,17] the possibility of at least transient carbon limitation, under highly enriched conditions, should not be ignored.[18] It should be noted that the Algal Assay Procedure Bottle Test, without modification, does not detect carbon limitation.

Table 1. Product moment coefficients of correlation (r) of parameters affecting productivity with yearly mean lake chl*a* concentrations. All data were converted to base 10 logarithmic expressions.

$\overline{\overline{\text{Par}}}$	All Lakes	All lakes with: RT <14 Days	RT ≥14 Days	Lakes with RT≥14 days and are: P-Limited	Transition	N-Limited	Stratified	Non-Stratified	Phyto-plankton Dominated	Macro-phyte Dominated
No. of Lakes	191	60	131	54	24	53	80	51	66	65
TP	0.74*	0.35*	0.84*	0.91*	0.84*	0.72*	0.80*	0.80*	0.88*	0.78*
DP	0.66*	0.28§	0.77*	0.85*	0.64*	0.65*	0.72*	0.72*	0.82*	0.67*
TP-DP	0.81*	0.50*	0.89*	0.92*	0.86*	0.79*	0.87*	0.85*	0.90*	0.87*
NH	0.48*	0.11	0.59*	0.76*	0.62*	0.23†	0.65*	0.48*	0.68*	0.41*
NO	0.26*	0.24†	0.33*	0.51*	0.49§	0.25†	0.17	0.45*	0.38*	0.28§
IN	0.42*	0.20	0.53*	0.71*	0.62*	0.25†	0.51*	0.51*	0.62*	0.35*
AL	0.37*	0.21	0.44*	0.42*	0.27	0.34§	0.48*	0.43*	0.58*	0.16
PH	0.49*	0.28§	0.58*	0.48*	0.21	0.65*	0.53*	0.54*	0.68*	0.38*
TP(AL)	0.71*	0.40*	0.78*	0.80*	0.70*	0.66*	0.73*	0.77*	0.84*	0.65*
T	0.30*	0.27§	0.33*	0.32§	0.51*	0.30§	0.23†	0.23†	0.24§	0.48*
RT	0.04	0.40*	-0.02	-0.15	-0.09	0.21	-0.18†	0.24†	0.08	-0.17
N/P	-0.51*	-0.21	-0.18§	-0.33†	0.04	-0.67*	-0.55*	-0.41*	-0.64*	-0.42*
SD[1]	-0.74* (178)	-0.40* (54)	-0.84* (124)	-0.87* (52)	-0.73* (23)	-0.75* (49)	-0.81* (80)	-0.77* (44)	-0.86* (63)	-0.76* (61)
TB[1]	-0.51* (186)	-0.12 (59)	-0.56* (127)	-0.51* (53)	-0.48§ (24)	-0.63* (50)	-0.15 (80)	-0.67* (47)	-0.55* (64)	-0.60* (63)

[1] Number of lakes given in parentheses.
*r significant at 0.01 level.
§r significant at 0.05 level.
†r significant at 0.10 level.

FACTORS AFFECTING PRODUCTIVITY

Chlorophyll *a* concentration (a measure of phtyoplankton biomass) was used as an index of productivity of the lakes sampled. Dillon and Rigler,[19] Jones and Bachmann,[20] and Bachmann and Jones,[21] and others have presented the strong relationship which exists between summer chl*a* levels and ambient TP concentrations measured at spring turnover, under summer conditions, or estimated from total inputs. The Dillon and Rigler[19] study lakes are Canadian shield lakes which undergo summer thermal stratification. Jones and Bachmann's[20] study lakes are mostly wind-driven systems in Iowa in which summer stratification, if any, is transitory. Regression equations for the two studies are quite similar, and each has a high coefficient of correlation. The summer chl*a*/TP relationship ($r = 0.95$) presented by Jones and Bachmann[20] is derived from a composite of their data and literature-cited data from 143 lakes covering a broad range of trophic states. The regression equation for the composite data is:

$$\log \mathrm{chl}a = -1.09 + 1.46 \log \mathrm{TP}\ (\mathrm{mg/m^3}). \quad (6)$$

If the phosphorus units are changed to mg/liter (our units), the comparable regression equation is:

$$\log \mathrm{chl}a = 3.29 + 1.46 \log \mathrm{TP}. \quad (7)$$

The regression equation for all 191 Survey lakes is:

$$\log \overline{\overline{\mathrm{chl}a}} = 1.78 + 0.57 \log \overline{\overline{\mathrm{TP}}}\ (r = 0.74) \quad (8)$$

Our equation yields lower chl*a* values per unit TP than the Jones and Bachmann equation given. The most likely explanation for this discrepancy is that the averaged seasonal chl*a* values used in generating our response equations underestimate the summer chl*a* maxima. To clarify the relationships of factors affecting productivity in the lakes sampled, a series of regressions was computed. The effects of phosphorus, nitrogen, total alkalinity, pH, light penetration, hydraulic retention time, nitrogen to phosphorus ratio, stratification, and phytoplankton versus macrophyte lake-domination were considered.

Retention times of the lakes were calculated using flow data provided by the U.S. Geological Survey (USGS) and known or estimated lake volumes. Where USGS flow data were not available, estimates of retention time were obtained from local or State agents familiar with the lake. Stratification was established using depth/temperature relationships from the Survey data and was verified or supplemented, where possible, by State personnel. An attempt was made to restrict "stratified lakes" to those which maintained a thermocline (minimum of 1° C change/meter depth) throughout most of the summer. Lakes exhibiting brief temporary stratification within the spring or summer periods were included as non-stratified. Information on phytoplankton- versus macrophyte-dominance was obtained from field observations, historical information, and contact with State and local personnel. Lakes which exhibited extensive reaches of submerged or floating higher aquatic plants, with histories of recurrent weed problems, and/or reported to be problem lakes in this regard were considered "macrophyte-dominated." Otherwise the lakes were included in the "phytoplankton-dominated" category.

The product moment coefficients of correlation (r) for the regressions are given in the table. The r values for all variables in the subpopulation of lakes with RT<14 are much lower than the corresponding r for lakes with RT>14, with the exception of RT itself. As the RT falls below 14, the relationship between chl*a* and variables weakens as RT is insufficient to reach potential biomass development. In studies by Payne[22] asymptotic levels for *Selenastrum*, *Anabaena*, and *Microcystis* were generally reached within 14 days after nutrient enrichment. The correlation of chl*a* with RT is better in short RT lakes; chl*a* development increases with time until it plateaus at about 14 days. The prediction of chl*a* for all lakes with RT>14 is:

$$\log \overline{\overline{\mathrm{chl}a}} = 1.95 + 0.68 \log \overline{\overline{\mathrm{TP}}} \quad (9)$$

with 71% of the variation in chl*a* being explained by changes in TP levels ($r = 0.84$; $r^2 = 0.71$).

Chlorophyll *a* correlations with DP mimic TP correlations but are lower in all subpopulations. Total phosphorus is highly correlated (r = 0.98) with DP and the regression equation is:

$$\overline{\overline{TP}} = 0.03 + 1.17\ \overline{\overline{DP}}. \qquad (10)$$

It is not surprising that the highest chl*a* correlations were with particulate phosphorus (TP-DP), as both are components of phytoplankton. The prediction equation for chl*a* for all lakes with RT$\geq$14 is:

$$\log \overline{\overline{chla}} = 2.36 + 0.75 \log (\overline{\overline{TP}}-\overline{\overline{DP}}). \qquad (11)$$

The ratio of $\overline{\overline{TP}}$-$\overline{\overline{DP}}$/$\overline{\overline{chla}}$ for 184 Survey lakes was 2.0, while Antia et al.,[23] working with marine phytoplankton, reported an average ratio of 1.8. The close agreement between the ratios indicates that TP-DP/chl*a* ratios are consistent between freshwater and marine communities. High mobility and short turnover times of phosphorus[24] through and between compartments within the general "phosphorus pool" make TP a good approximation of bioavailable phosphorus.

Of the forms of nitrogen examined, NH was found to be most strongly correlated with mean chl*a*. This positive correlation is strongest in the P-limited (r = 0.76), declines in the transition (r = 0.62), and is very weak in the N-limited lakes studied (r = 0.23). This pattern of decline is also noted with NO and IN.

That the relationships between the dissolved nitrogen forms tested and mean chl*a* decline dramatically as we move from P- to N-limited lakes is somewhat of a paradox. It is not unreasonable to expect higher correlations between a nutrient and biological response as that nutrient exerts a greater degree of limitation on the biological response, e.g., the phosphorus relationship. A possible explanation for this apparent contradication is increased fixation of atmospheric nitrogen by blue-green algae. The N-limited lakes studied were generally nutrient rich. An increase in the frequency of *Anabaena* or *Aphanizomenon* blooms (both nitrogen-fixers) in association with nutrient enrichment is consistent with general observations in the aquatic literature. Short RT lakes show very weak relationships between the nitrogen forms examined and chl*a*. The relationship with respect to NO does not appreciably improve in longer RT lakes, but improves substantially for NH. It should be noted that similar processes often produce parallel increases in phosphorus and NH within the hypolimnion.

The relationship of PH to chl*a* was found to be much stronger in phytoplankton- than in macrophyte-dominated lakes (r = 0.68 versus r = 0.38). The weak relationship in the latter group is not unexpected, as no attempt was made to quantitatively sample macrophytes or their associated chl*a*. The PH increases with the removal of carbon dioxide (CO_2) by photosynthetic activity. It should be noted that phytoplankton utilization of CO_2 per unit volume (and hence the corresponding PH change) has been reported to be 10 times as high as macrophytes.[25] The differences noted in short and long RT lakes (r = 0.28 versus r = 0.58) suggest that diurnal CO_2 changes alone do not explain the PH/chl*a* relationship.

The relationship between AL and chl*a* is, once again, much stronger in phytoplankton- than macrophyte-dominated lakes. In general, increased AL and nutrient enrichment go hand in hand. However, the degree and nature of macrophyte "dominance" and its effects upon nutrient reduction (competition with phytoplankton), shading (submerged versus floating macrophytes), etc., result in a broad scatter of chl*a* values and generally weak relationship.

The two-factor parameter TP(AL) is used to assess to what degree the "unit response" (chl*a* per unit TP) is a function of AL levels. Addition of AL did not improve the basic chl*a*/TP relationship; the correlations were slightly lower throughout the lake groups examined.

Chlorophyll *a* response as a function of N/P ratio was found to be much stronger in N- than P-limited or transition lake groups (r = 0.67 vs. r = 0.33 or r = 0.04). As phosphorus levels increase, the N/P ratio generally decreases and chl levels increase. This is consistent with our observation that the N-limited lakes examined were generally high in phosphorus.

Edmondson[26] found a negative hyperbolic relationship between SD and chl*a* concentrations in Lake Washington. We found SD and TB to be negatively correlated with chl*a*. The largest difference between SD and TB correlations (r = -0.81, r = -0.15, respectively) occurred in the stratified lakes. A likely explanation is that TB values were averaged through the entire water column and include a greater percentage of "clear" waters from below the euphotic or epilimnetic zones in stratified lakes. The strongest correlation was noted in non-stratified lakes where TB values represent measurements taken within the effective mixing zone. These relationships suggest that the bulk of photic zone turbidity in the stratified lakes sampled was of phytoplankton origin.

The correlations for various chemical and physical parameters, with the exception of NH and NO, are quite similar in stratified and non-stratified lakes. The NH correlation with chl*a* is higher in stratified lakes than in non-stratified lakes; the reverse is true for NO. A possible explanation for this is that under reducing conditions, such as hypolimnetic deoxygenation, NH and phosphorus are concomitantly released. In non-stratified lakes the prevalent inorganic nitrogen component is nitrate-N.

Most correlations of chl*a* with chemical and physical parameters are higher in the phytoplankton-dominated subpopulation than in the macrophyte-dominated subpopulation. The contribution of macrophyte chl*a* was not measured, and no information on the relative quantities of submerged versus floating weeds is available for Survey lakes. Many submerged aquatics, with little reliance on ambient nutrient levels in the water, can survive on nutrients absorbed through their root systems. However, free-floating macrophytes and phytoplankton have similar ambient nutrient requirements. The prediction equations for all phytoplankton-dominated lakes with RT>14 are:

$$\log \overline{\overline{chla}} = 1.91 + 0.68 \log \overline{\overline{TP}}, \text{ and} \qquad (12)$$

$$\log \overline{\overline{chla}} = 2.31 + 0.73 \log (\overline{\overline{TP}}-\overline{\overline{DP}}). \qquad (13)$$

STUDIES IN PROGRESS

Other aspects being investigated include the effects of additional parameters on productivity, the intercorrelation of parameters affecting productivity, effects of lake use upon water quality "suitability," effects of manifestations of nutrient enrichment on water use, and prediction of lake condition from ambient and loading conditions.

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APPLICATIONS OF THE SINGLE SOURCE (CRSTER) MODEL TO POWER PLANTS: A SUMMARY

Joseph A. Tikvart*
Connally E. Mears
Source Receptor Analysis Branch
Office of Air Quality Planning and Standards
U.S. Environmental Protection Agency
Research Triangle Park, N.C.

*On Assignment from the National Oceanic
and Atmospheric Administration (NOAA)

Summary

For the last three years the Environmental Protection Agency has conducted a series of atmospheric dispersion model studies of power plants. These studies have considered the impact of approximately 700 utility power plants whose generating capacity is 25 megawatts or greater. Included in these studies are (1) dispersion model estimates of SO_2 concentrations downwind from each power plant, (2) validation of the Single Source Model with data for several typical power plants and (3) a sensitivity analysis of this model. The results of these studies have been used effectively in a number of energy/environmental policy considerations. This paper summarizes the findings of the various studies.

Introduction

Shortages in the availability of low-sulfur fossil fuels have been given national prominence. These shortages are particularly significant to utility power plants for two reasons: (1) power plants typically use large quantities of fossil fuels and (2) many of the State Implementation Plans (SIPs) require severe reductions in sulfur dioxide emissions from power plants which burn fossil fuels. The shortage of low-sulfur fuel necessitates the elimination of unduly stringent SIP control regulations, where this can be done without endangering air quality standards. The fuel shortage has also led to legislation which empowers the Federal Energy Administration to require that specific power plants switch from oil or gas to coal. This switch to coal, however, cannot be allowed to result in a threat to air quality standards. Furthermore, to meet the Clean Air Act requirement for attainment and maintenance of acceptable air quality, it may be necessary to revise the SIPs for selected source categories, including power plants. The power plant studies summarized in this paper support actions like those noted above.

Estimates of the air quality impact caused by power plants are major components of these studies. A dispersion model is a commonly used technique for relating pollutant emissions to ambient air quality. It is a mathematical description of pollutant transport, dispersion, and transformation processes that occur in the atmosphere. The Single Source (CRSTER) Model is the primary dispersion model applied in all the power plant studies discussed in this summary paper.

Due to severe time constraints and the fact that models like the Single Source Model are widely applied and considered state-of-the-art, the accuracy of this model was not analyzed in the initial phase of the power plant studies. However, some analyses of the Single Source Model have been recently completed and others are continuing. These include validation studies, sensitivity analysis and model improvement.

Following sections of this paper discuss (1) the Single Source Model, (2) power plant studies in which it is applied, (3) evaluation of the model through validation and a sensitivity analysis, and (4) applications to energy/environmental policy considerations.

Single Source (CRSTER) MODEL

The Single Source (CRSTER) Model is a Gaussian plume model. It is based on the dispersion coefficients and equations described by Turner[1] and on the plume rise equations described by Briggs[2]. The model is essentially the same as that discussed by Hrenko et al[3]. It is designed to estimate concentrations for averaging times of 1 hour, 24 hours, and 1 year due to sources at a single location. The concentrations are estimated for a circular array of receptor sites which are located so as to approximate the downwind distances at which the highest concentrations are likely to occur.

The model estimates concentrations for each hour of a year, based on wind direction (in increments of 10 degrees), wind speed, Pasquill stability class, and mixing height. Meteorological surface data for 1964 are frequently used in the power plant studies, although, with the proper data, any year could be used. The reasons for the routine use of 1964 meteorological data are (1) data from earlier years do not have an adequate resolution of wind direction, and (2) data from subsequent years are not readily available on an hourly basis. Mixing height data are from the upper air observations made at selected National Weather Service stations. Hourly mixing heights are estimated within the model by use of an objective interpolation scheme. Decay of the pollutant between source and receptor is ignored.

To simulate the effect of elevated terrain in the vicinity of plant sites, a terrain adjustment procedure is used. This procedure decreases the effective plume height by an amount equal to the difference in elevation between the plant site and the specific receptor site. The model then uses the adjusted plume height in estimating concentrations at that receptor. In those cases where terrain features are found to be greater than the effective plume height of the plant, the Single Source Model is not applied.

Power Plant Studies

Purpose and Limitations

The power plant studies have considered the impact of approximately 700 utility power plants whose generating capacity is 25 megawatts or greater. The studies may be divided into three parts. These are analyses for (1) the feasibility of compliance extensions in 51 selected Air Quality Control Regions (AQCRs), (2) the feasibility of oil-to-coal conversions at selected power plants and (3) the general impact of power plants on ambient SO_2 concentrations in 128 AQCRs. In all cases the studies are primarily concerned with estimates of the maximum 24-hour concentrations of SO_2. This averaging time and this pollutant are the critical ones for which power plants must meet primary National Ambient Air Quality Standards (NAAQS). The second study is the only one which considers particulate concentrations. Also, in those cases where it is estimated that neighboring power plants could contribute concentrations which add to those caused by the plant under consideration, an interaction analysis is performed.

All source data used in the power plant studies are taken from the Federal Power Commission (FPC Form 67) for base years of 1971 or 1972. In those cases where emissions are projected to 1975, appropriate data are taken from "Steam Electric Plant Factors"[4].

Emissions data are based on average monthly operations for each month of the year; such monthly data are the limit of detail routinely available from the FPC. A power plant could quite possibly operate at near-maximum rated capacity for 24 hours, which would not be apparent from the monthly data. If these operations were coincident with days of poor dispersion conditions, the estimated maximum concentrations could be significantly low. Thus, two sets of emission conditions are routinely considered. One is the nominal load case in which average hourly emission rates are used; they are assumed to be constant, except for variations by month. The other is the maximum load case where emissions and plume rise are based on the plant continuously operating at 95 percent of rated capacity. Both sets of emissions data are considered and the one which results in the highest estimated concentrations is used.

It should be noted that any use of these studies must recognize the inherent limitations resulting from the data and procedures used in the modeling effort. Before final judgment on the control of specific plants is made, other factors, not addressed in these studies, should be considered. These include: the impact of other sources in the area, projected growth in the area, measured air quality data, known or suspected downdraft or fumigation problems, unique nearby terrain features, nearby land use patterns and population distributions, more specific operational data for the plant, impact of new units, specific meteorological studies for the area, and additional studies or findings by other investigators.

Compliance Extension Studies

In 1972 a study by EPA on the aggregate demand created by the SIPs for low-sulfur coal was conducted. This study indicated a nationwide potential deficit of about 100 million tons/year of such coal by 1975. The deficit was considered most acute in 12 states with high coal consumption rates. One means to alleviate the deficit would be to selectively reduce the requirements for low-sulfur coal in those cases where a higher sulfur coal could be used without endangering the NAAQS.

An initial modeling study of SO_2 emissions in several AQCRs had been conducted. This study showed that some of the large power plants could be temporarily allowed to burn coal at 1970 sulfur levels without threatening the 24-hour NAAQS. Based on the results of this study, it was decided to consider selected power plants in 12 states which are heavily dependent on coal. This involved a total of approximately 200 power plants in 51 AQCRs.

The study[5,6] finds that at approximately 55 percent of the plants considered, some relaxation of emission limitations is possible. Relaxation could result in increasing the average allowable percent sulfur content of fuel from approximately 1 percent sulfur content to 2 percent sulfur content at the plants considered. Thus, the projected deficit in low-sulfur coal could be eliminated.

Fuel Conversion Studies

The compliance extension studies discussed in the preceding section had been conducted prior to the overall oil shortage and energy crisis which became apparent in late 1973. The oil shortage initiated a second study of selected power plants on the U.S. East Coast. In this second study[7,8], fuel conversion from oil to coal for selected boilers within specific plants is analyzed to evaluate the impact on SO_2 and particulate concentrations. Increased SO_2 emissions due to fuel conversions at 16 of 43 plants considered are estimated to result in concentrations from the plants alone which exceed the 24-hour NAAQS. Seven of the plant conversions are estimated to result in concentrations from the plants alone which exceed the 24-hour particulate NAAQS. The analysis indicates that in some cases partial conversion from oil to coal at selected power plants appears to be a viable option for alleviating the East Coast oil shortage.

Studies of Power Plants in 128 AQCRs

Further studies[9,10] of about 400 power plants distributed throughout the U.S. have been conducted in 1974 and 1975. The purpose is twofold: (1) to complete, on a national basis, analyses of the threat of large emitters of SO_2 to the NAAQS and (2) to add to the overall analysis of the power plant industry being conducted by governmental agencies and industry itself. Thus, a base for further analyses is developed and is available if additional decisions must be made concerning general EPA policy on compliance extensions or fuel use options for power plants. Of these 400 additional plants it is found that nearly 20 percent currently may exceed, by themselves, the 24-hour SO_2 air quality standards.

Evaluation of Model

Validation Studies

To determine the validity and overall accuracy of the Single Source Model, validation studies have been performed for the Canal, Paradise, Philo, Stuart and Muskingum River power plants. The Canal Plant[11] is located in Massachusetts along Cape Cod Bay. The Paradise Plant[12,13] is located in Western Kentucky. The other three plants are located in Southern

Ohio[14,15]. In all cases, hourly variations in SO_2 emissions are determined for each plant. These emissions are then used with hourly meteorological data which are representative of transport and dispersion in the vicinity of the plant. These data are input to the model and 1-hour, 3-hour, 24-hour, and annual concentration estimates are made for the sites at which air quality monitors are located. The estimated and the observed concentrations are then subjected to several statistical comparisons. These include comparisons of highest and of second-highest concentrations and comparisons of observed and estimated concentration frequency distributions.

As shown in Table 1, the model generally tends to underestimate the highest and the second-highest 24-hour average concentrations. This is also true for 3-hour average concentrations. However, 1-hour averages are equally divided between overestimates and underestimates. In cases where surrounding terrain is nearly as high as the stack top (see the Philo Plant in Table 1), the model overestimates concentrations for all averaging times. It should be noted that most dispersion models comparable to the Single Source Model are not truly applicable in the vicinity of such significant terrain features.

Table 1. Comparison of Observed and Estimated Concentrations (µg/m³).

		1-Hour Average Concentrations				24-Hour Average Concentrations			
		2nd Highest		Highest		2nd Highest		Highest	
Plant	Sampling Station	O[a]	E[b]	O	E	O	E	O	E
Canal	1	435	253	438	283	66	16	75	29
	2	553	174	618	179	36	9	46	11
	3	446	446	732	509	77	38	83	39
	4	575	427	638	479	63	4	75	16
Stuart	1	685	1372	857	1393	259	149	277	161
	2[c]	685	814	1014	948	63	75	159	98
	3	1022	565	1153	1022	181	91	225	102
	4	750	515	883	541	79	45	83	49
	5	495	823	565	1219	63	57	77	75
	6	980	595	1053	693	147	69	195	83
	7[c]	325	976	435	1000	69	73	77	120
Muskingum River	1	857	980	925	1083	133	81	170	97
	2	786	1304	786	1310	131	82	137	91
	3	996	873	1179	933	165	73	227	74
	4	735	465	786	645	109	45	115	47
Philo	1	525	1295	893	1639	132	133	133	147
	2	735	945	891	1059	67	86	110	104
	3	745	4049	917	4593	127	471	132	541
	4	665	1945	695	1981	62	165	158	220
	5	575	1279	675	1344	87	222	94	226
	6	565	2359	595	2482	121	282	138	356

[a] Observed concentrations with subtracted background.
[b] Estimated concentration.
[c] Samplers were in operation for less than half the year.

In the comparison of observed and estimated frequency distributions, disparate results are found. There is considerable variation in comparisons from site-to-site and plant-to-plant. However, agreement improves for frequency distributions which include all monitoring sites around a particular plant. As shown in Figure 1, all but the few highest and lowest concentration percentiles are accurately estimated for the distributions which include all sites.

Until further studies become available, it may be concluded from these validation studies that the Single Source Model is generally accurate within a factor of two. This is not surprising since this accuracy is widely accepted for such point source models. However, an important element is identification of the tendency to underestimate, rather than overestimate, concentrations for averaging times associated with NAAQS. This tendency undercuts the position of those who contend that such models are overly conservative when used in determining emission control requirements. It also places an added burden on pollution control officials to ensure that an environmental threat is not understated.

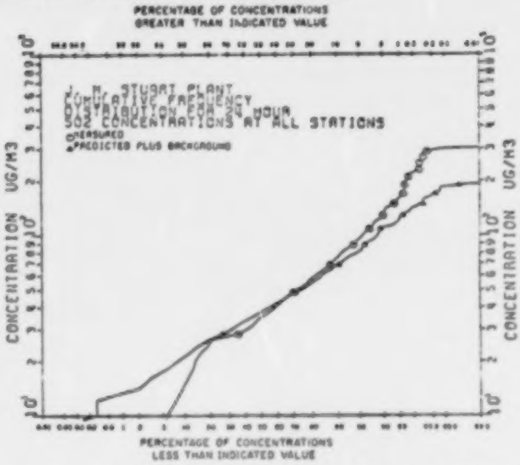

Figure 1. Stuart Plant Cumulative Frequency Distrbution for 24-Hour SO_2 Concentrations at All Stations.

Sensitivity Analysis

To further understanding of the behavior of the Single Source Model, a sensitivity analysis[16] has been conducted. Specifically, this analysis examines the impact of variations or errors in the input data on the concentration estimates produced by the model. Thus, it identifies the model parameters which have the greatest influence on concentration estimates.

In the analysis the incremental change in predicted concentration is determined for an incremental change in input. A case study approach is used with the three Ohio power plants noted above. The analysis is limited to the maximum estimated 24-hour concentration, since this is generally considered to be the most important averaging time for power plants with regard to primary air quality standards.

Both source parameters and meteorological parameters are considered. The source parameters are (1) stack height, diameter, gas exit velocity, and gas exit temperature, (2) emission rate and its monthly variation and (3) terrain adjustment. The meteorological parameters considered are mixing height, wind speed, ambient temperature and stability class. With the exception of stability class, each parameter is varied by a factor of ± 5, ± 10, and ± 25 percent while all other parameters are held constant.

From the analysis summarized in Tables 2 and 3, it is found that for sources with relatively short stacks, for example the Philo Plant which has stacks about 300 feet high, a percent change in any stack parameter results in at least that percent change in the maximum 24-hour concentration. For sources with relatively tall stacks, for example the Stuart Plant which has stacks about 800 feet high, a lack of such sensitivity is found. Stability class, a meteorological parameter, is found to be a highly sensitive factor for all plants, since this parameter can take on only six discrete values. The importance of parameters such as wind speed and mixing height varies depending on the meteorological conditions that result in highest concentrations for a plant. In all cases, the percent change in the maximum 24-hour concentration is less than the percent change in these meteorological parameters. Tables 2 and 3 indicate percent changes in maximum 24-hour concentrations for positive variations in source and meteorological parameters. Comparable changes in concentration can also be shown for negative variations in these parameters.

Table 2. Percentage Change From Base Case-- Maximum 24-Hour Concentrations Due to Variations in Source Related Parameters.

Percent Variation in Parameter / Parameter	Muskingum River			Philo			Stuart		
	+ 5	+10	+25	+ 5	+10	+25	+ 5	+10	+25
Stack height (m)	-2	-5	-11	-6	-12	-27	-2	-5	-11
Stack temp (°C)	-4	-8	-17	-4	- 8	-18	-2	-4	- 7
Exit velocity(m/s)	-5	-9	-19	-6	-10	-23	-2	-3	-7
Stack diameter(m)	-11	-17	-30	-11	-20	-43	-3	-6	-15
Terrain ADJ (m)	1	3	12	5	9	24	1	1	3
Emissions(gm/sec)	5	10	25	5	10	25	5	10	25

Table 3. Percentage Change From Base Case-- Maximum 24-Hour Concentrations Due to Variations in Meteorological Parameters.

Percent Variation in Parameter / Parameter	Muskingum River			Philo			Stuart		
	+ 5	+10	+25	+ 5	+10	+25	+ 5	+10	+25
Mixing height (m)	0	0	0	0	0	0	-3	-5	-11
Wind speed (m/s)	3	5	9	4	7	21	-2	-3	-9
Ambient temp (°C)	1	2	6	1	2	6	1	2	5
Stability class*	-	-	-43	-	-	-40	-	-	-47

*Biased by +1 Stability Class

The sensitivity of the maximum estimated concentrations to changes in meteorological data sets is also determined. Three data sets are used with each set of source data. Changes in maximum concentration from the base case which are shown in Table 4, range from an increase of nearly 50 percent to a decrease of almost 30 percent. Inherent in the change of maximum concentration are the effects of the wind direction and the variability of wind direction. These are not considered individually in the sensitivity analysis. However, wind direction and its variability, which are a function of the meteorological conditions peculiar to each data set, play a major role in the percent concentration changes shown in Table 4. This illustrates the importance of a meteorological data set which is as representative of transport and dispersion in the vicinity of the plant as possible.

As a result of this analysis it can be concluded that: (1) the sensitivity of model estimates to accuracy in the input parameters varies from source to source; (2) accuracy in the source parameters becomes more critical as the stack becomes shorter; (3) errors in individual meteorological parameters, with the exception of stability class, result in somewhat smaller errors in estimated concentrations; (4) the cumulative errors in meteorological parameters, which result from the use of data from an unrepresentative site, can cause substantial errors in estimated concentrations.

Table 4. Percentage Change From Base Case--Maximum 24-Hour Concentrations Due to Variations in the Meteorological Data Sets.

Surface/Upper Air Data Set	Muskingum River	Philo	Stuart
Huntington/Huntington	-	-28.4	-19.4
Columbus/Dayton	47.8	-	36.0
Cincinnati/Dayton	11.6	-5.8	-

Model Improvement

As a result of the model validation and the sensitivity analysis, studies to improve the Single Source Model are being undertaken. Two specific areas under investigation are (1) the use of other stability classification and dispersion parameters which may allow better estimates of plume dilution and (2) the use of more precise information on the stack parameters which affect plume rise. Also, additional analyses are being undertaken to evaluate the accuracy of hourly concentration estimates for various meteorological regimes. The goal is to assess the need for better data inputs or more precise algorithms in the model. Based on these studies, improvements in the model will be considered.

Applications of Power Plant Studies

Limitations on the model and its application in the power plant studies have been noted. Even with these limitations, the power plant studies are of value for use in generalized analyses which assess the overall effect of some plan of action for the utility industry. These studies have been used effectively in a number of energy/environmental policy considerations.

The Clean Fuels Policy is an EPA program to encourage some states to eliminate unnecessarily stringent control regulations in their SIPs and thereby alleviate the shortage of low sulfur coal. The power plant studies demonstrated the potential usefulness of such a policy and helped to indicate those SIPs where unnecessarily stringent regulations might exist.

The power plant studies were used in early analyses of proposed oil-to-coal conversions. They were useful in indicating the types of sources which were good candidates for conversion and specifically indicated several plants that were poor candidates. These studies have been used for roughly assessing the allowable percent sulfur coal which could be used in oil-to-coal conversions required under the Energy Supply and Environmental Coordination Act. They will serve as a basis for more detailed subsequent analyses.

In the development of EPA policy on tall stacks and meteorological control systems, the power plant studies were used frequently. They were used to analyze alternatives for limitations on stack height increases. They allowed the frequency and amount of emission reductions that would be required by meteorological control systems to be compared, for various categories of power plants, to permanent control requirements.

The power plant studies have been the basis for analyses in support of a viable SO_2 control strategy for Ohio. They were used as justification for existing regulations in the 1974 Ohio SO_2 hearings. They were used as an initial base in developing EPA Region V's current proposed regulations for Ohio[17]. They have also been used by Region IV in the development and revision of SIPs applicable to power plants located in the Southeastern United States.

Industry has used the power plant studies in statements[18] to the U.S. Congress on options for control of SO_2. These studies have also been used in evaluating the impact of proposed legislation to prevent significant deterioration of air quality.

Based on the demand for the reports resulting from such power plant studies, it is logical to conclude that other regulatory agencies and industrial groups are using these studies. In most cases, they are being extended by more detailed analyses. It appears that these studies will continue to play an important role in the development of regional and national environmental policies which affect utility power plants.

Acknowledgments

The authors wish to recognize the major contributions of their co-workers to these power plant studies. Major contributions were made by D. Barrett, W. Freas and R. Lee under the overall direction of H. Slater. Special recognition is also due to those individuals who performed the bulk of the work under contract to EPA. These include: P. Morgenstern and L. Morgenstern of Walden Research Division of Abcor, Inc.; R. Koch of GEOMET, Inc.; and M. Mills and R. Stern of GCA Corporation. Thanks are also due to Mrs. B. Stroud who diligently prepared this manuscript.

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MODIFIED DISPERSION MODELING PROCEDURES FOR INDIANA POWER PLANTS

S. K. Mukherji, Chief
Program Support Branch
Indiana Air Pollution Control Division
Indianapolis, Indiana

M. W. Bobb
Program Support Branch
Indiana Air Pollution Control Division
Indianapolis, Indiana

C. R. Hansen
Program Support Branch
Indiana Air Pollution Control Division
Indianapolis, Indiana

H. D. Williams
Director
Indiana Air Pollution Control Division
Indianapolis, Indiana

David R. Maxwell
Standards & Planning Branch
Indiana Air Pollution Control Division
Indianapolis, Indiana

Summary

A modified procedure for short-term dispersion modeling of Indiana power plants located along river valleys is presented in this study. Rough terrains and occasional high winds persistent for hours produce high surface turbulence in this particular region. Based on empirical observations, the meteorological stability input to the PTMTP modeling program of the UNAMAP package was appropriately decreased. The artificial stability change simulated the augmented atmospheric turbulence due to surface friction. Generation of more accurate sulfur dioxide level estimates indicated the feasibility of using conventional short-term models with suitable changes in particular cases.

Introduction

A modified procedure for short-term sulfur dioxide dispersion modeling of four Indiana power plants located in the Ohio River & Wabash River valleys is presented in this study. These river valley regions are characterized by undulating hills and bluffs at some distance from the river and occasionally persistent strong winds blowing across the river towards the rough terrain. The basic assumptions incorporated in the available simulation models for atmospheric transport of SO_2 do not account for this type of situation. As a result, the conventional short-term dispersion models, viz., the programs included in United States Environmental Protection Agency's modeling package consistently underpredicted maximum SO_2 levels around the power plant. A simple change involving meteorological parameter inputs to the computer model was, therefore, initiated to simulate the actual atmospheric conditions more closely and generate more accurate estimates, using conventional modeling programs.

The particular UNAMAP package model targeted for modification was the Multiple Point Source routine PTMTP[1] (also identified as DBT51). In this program the usual simplifying assumptions are made; namely, steady and uniform meteorological conditions with no wind direction shear, Gaussian Plume behavior, flat or gently rolling terrains, no aerodynamic downwash conditions, etc. One important and desirable feature of PTMTP is that an hourly stability condition can be assessed by a meteorologist from the available ambient data before being input to the model. Since the local topography and wind data suggested the possibility of considerable mechanical turbulence generation, the stability class evaluation was isolated as the program area suitable for prediction improvements. The analytical considerations that led to hourly stability postulations are now described.

Analytical Background

A theoretical treatment of the effects of an extensive area of given roughness on the short-range vertical spread from a source, using gradient-transfer methodologies, has been available for some time.[2] Influences of terrain roughness changes on pollutant dispersions have also been detailed by Pasquill, et al.[3, 4, 5] Expectedly, moderately rough terrains, i.e., ridges and valleys seem to cause strong mixing.[6, 7, 8] This mixing pattern is usually prominent during late morning hours under slightly unstable conditions of the atmosphere and compares favorably with thermally induced stability alterations. It is true that low-level (less than 100m) sources within a confined narrow valley sometimes do not reflect any mechanical mixing.[9] However, it is generally acceptable that local atmospheric turbulence can be greatly increased, at least, within the lower 500 to 1000 meters of the atmosphere through surface friction effects.[3]

Counihan[10] studied average strong wind or neutral boundry layers and concluded their appropriate depth to be about 600 meters. He proposed an expression for surface friction velocity u_o^* as follows

$$u_o^* = (U_g/20)(\ 1 + 0.24 \log (z_o/0.38))^{1/2} \qquad (1)$$

In this equation, U_g denotes the geostrophic wind speed and z_o represents the characteristic surface roughness. For wooded rural terrain, Counihan cites a value of $z_o = .38$m. Rougher terrains encountered in the Ohio River or Wabash River Valley regions of Indiana can be presumed to possess surface roughness eqivalent to approximately 0.58m. In other words, the friction velocity for the Indiana study ranges from $0.050U_g$ to $0.051\ U_g$. A theoretical analysis by Wipperman[11] suggests that the boundary layer depth is about $0.8\ ku_o^*/f$ falling to $0.2\ ku_o^*/f$ under very stable conditions (where f, the Coriolis parameter approximately equals 10^{-4}/s and k is the dimensionless Von Karman's constant = 0.4). Thus the mesoscale boundary layer depths h in the vicinity of the power plants vary from $160U_g$ to $163U_g$ for so-called neutral stabilities. The value of h decreases to about $40U_g$ in very stable conditions. Translated in terms of numbers, the boundary layer can extend to about 800m for sustained windspeeds greater than 5 m/s typically encountered in the area.

Dispersion in a mechanically stirred boundary layer has been discussed by Moore.[12] According to the analysis, maximum diffusivity within a boundary layer is expected to occur at around h/4 corresponding to 200m height on windy days. Indiana power plant stacks under study are well below the depth of 200m. Therefore, any plume behavior on these days is expected to be significantly affected by the mechanically induced turbulence in the atmosphere. The effects of higher turbulence on the SO_2 plume were simulated in the PTMTP model by reducing the atmospheric stability by one class from the conventional one when the situation dictated so. The algorithms for the stability reduction are described below.

Modeling Modification

To begin with, preliminary topography and wind direction surveys were carried out for the individual power plant to be modeled. The purpose was to ascertain the magnitude of terrain roughness changes within 5 km of the plant and its likely effects on the plume rise and spread. Next, a set of guidelines was laid down to establish the likelihood of strong friction-generated turbulence interacting with the plume. This consisted of scanning (a) the elevation changes around the plant and (b) the hourly meteorological data, namely, time of day, season, cloud cover, wind speeds, etc. Upon the set of pre-established criteria being met, the conventional stability class (based on Pasquill-Gifford-Turner suggestions) was decreased by one. Thus, if during summer daytime the windspeed was greater than 4 m/s with the sky being at least partly clear, the stability class was lowered by one provided the wind was blowing the plume over the rough terrain. The flow chart leading to the synthetic decrease of the stability parameter as input to the PTMTP model is indicated in Figure 1.

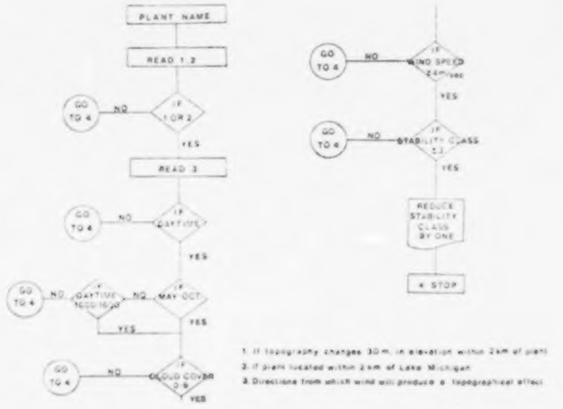
PLANT NAME
READ 1,2
GO TO 4
NO
IF 1 OR 2
YES
READ 3
GO TO 4
NO
IF DAYTIME
YES
GO TO 4
NO
IF DAYTIME 1000-1600
NO
IF MAY-OCT
YES
YES
GO TO 4
NO
IF CLOUD COVER 0-6
YES
GO TO 4
NO
IF WIND SPEED ≥4m/sec
YES
GO TO 4
NO
IF STABILITY CLASS ≥3
YES
REDUCE STABILITY CLASS BY ONE
4 STOP
1. If topography changes 30 m. in elevation within 2km of plant
2. If plant located within 2 km of Lake Michigan
3. Directions from which wind will produce a topographical effect

Figure 1. Flow Chart to Assess Stability Alterations

It is noted that no change of stability was allowed for classes 1 and 2. Turbulence generated by thermal instability associated with these two classes was assumed to be much more dominant compared to dynamic turbulence production.

Results

Typical elevation changes around two of the power plants are presented in Figures 2(a) and 2(b). Figure 2(a) depicts a sudden 110m jump in elevation at a distance of 6 to 12 stack heights from the source, i.e., a step change in the floor level of the flow. A more modest elevation increase is seen in Figure 2(b), where the elevation changes may be construed as rough elements embedded at the lower boundary of the surface layer flow.

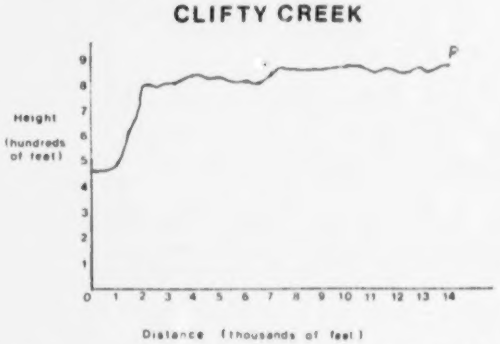

Figure 2(a). Elevation Changes at Clifty Creek Plant

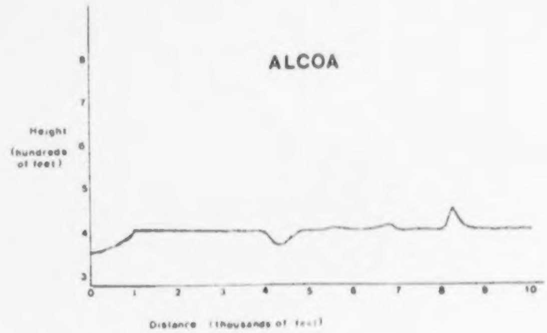

Figure 2(b). Terrain Roughness Around
Warrick-Culley Units

In both cases, an artificial change of stability for any flow over the elevated terrain generated more accurate estimates.

Comparisons of the actually monitored sulfur dioxide readings with the levels projected by the lowered stability input to the PTMTP model are compiled in Table 1 on the following page.

TABLE 1. Comparison of Actual Reading Versus 24-Hour Predictions (ug/m^3)

Point Source	Conventional Stability Assumptions	Altered Stability Assumptions	Actually Monitored SO_2 Reading
Warrick-Culley	226	435	479
	17	368	479
	126	532	506
	97	336	275
Clifty Creek	0.002	126	29
	0.3	49.6	20
Wabash River	23	31	31

Assessments of the SO_2 levels using conventional stability assumptions are shown side by side. The results reflect the days when persistent strong winds were measured flowing over the rough terrains. In both sets of computations, the actual elevation of the receptors was taken into account. It should be noted that the Warrick-Culley monitors/receptors were generally very close to the plume centerline during the days of study. On the other hand, the monitors for the Clifty Creek and Wabash River plants were located kilometers away from the estimated maximum SO_2 impact sites. For the low-level ranges of SO_2 indicated by the monitors, the accuracy of the equipment was within 10 percent of the observed readings at best. Finally, the background SO_2 levels over the river valley basins are estimated to be around 10-25 ug/m^3 on the basis of acquired data and wind persistence studies.

Typical alterations in SO_2 isopleths when the stability classes were decreased are portrayed in Figures 3(a) and 3(b) for two power plants.

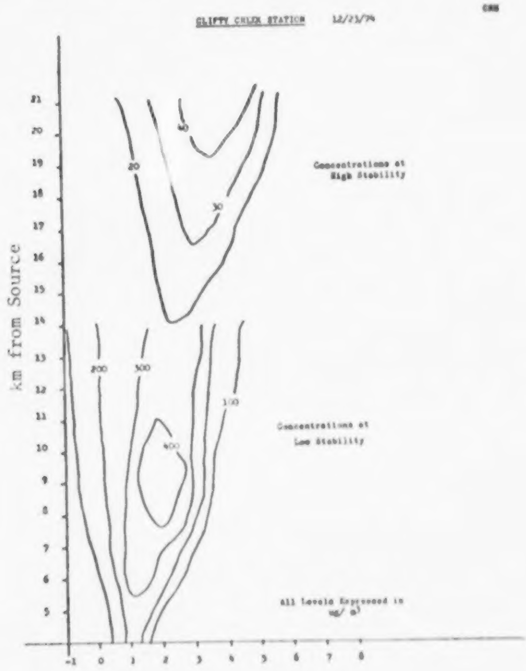

Figure 3(a). Isopleths for Projected Levels Around Clifty Creek Plant

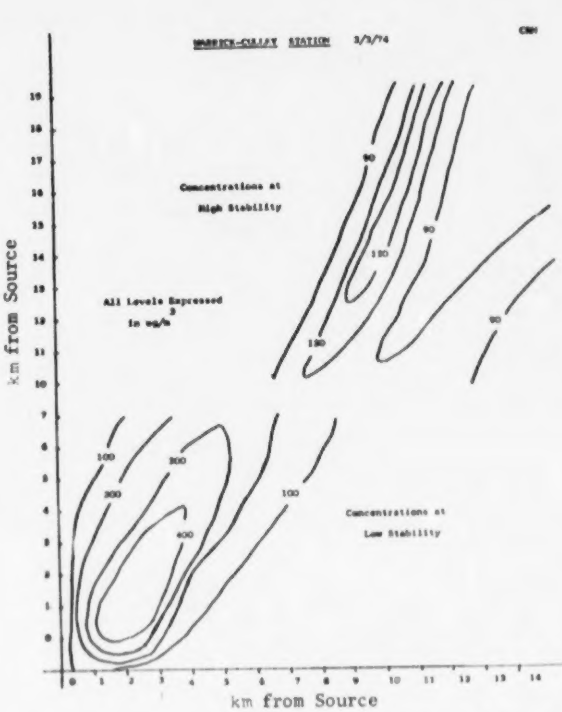

Figure 3(b). Estimated SO_2 Impacts of Warrick-Culley Stations

Displacements of the maximum impact locations caused by the meteorological changes are clearly discerned. It is also evident from these figures that the effects of stability changes drop off sharply from the maximum impact location. At a distance of 3-5 kilometers away from the maximum SO_2 level region, the difference between the two estimates becomes negligible. The minor differences between the numerical SO_2 estimates for Clifty Creek and Wabash River monitor/receptors are attributable to this effect. In view of these considerations, it is reasonable to propose that the actual stability parameters estimate the pollution levels somewhat better than the conventional stability inputs.

To substantiate this statement further, a detailed review of resuls obtained from the Warrick-Culley Power Plant complex is presented in Table 2.

TABLE 2. Comparison of Estimated SO_2 Levels Near Warrick-Culley Plants

Monitor	Monitor Location	Obs. 24-hr SO_2 Level (ug/m^3)	24-hr SO_2 Level Estimates (ug/m^3) (includes background levels) Lower Stability	Higher Stability
		472	421	30
P2	2.9 km.	472	365	26
		83	222	162
		131	99	60
		104	120	69
P1	3.7 km.	52	26	134
		20	30	31
P3	3.0 km.	52	26	133
M1		208	151	26
(Mobile Site)	0.95 km.	314	126	26

These results represent days on which high levels of SO_2 were projected to occur at or near one of the operating samplers due to direct impact. Such a choice of days tended to provide a more valid comparison between the two estimates (based on different hourly stability parameters), since the uncertainty effects for off-axis plume concentration predictions were less significant. It is seen from the results that the lower stability assumptions generated more accurate projections for nine out of ten days. Within this duration the total number of hours for which stability levels were artificially decreased by one class exceeded one hundred. An hourly correlation analysis between the actual readings and the two estimates yielded low values for the coefficient 'r', i.e. 'r' was less than 0.40. However, the analysis spanning this period indicated better regression results for the lower stability cases. The lesser SO_2 estimates for the nearby monitor M1 probably resulted from inaccurate wind direction assessment for the two days.

In the overall analysis, forced lowering of stability to represent a more turbulent flow field provided a more accurate assessment of the samplers. On the basis of results presented it is suggested that similar procedures be routinely incorporated in any dispersion modeling scheme where dominant mechanical turbulence effects are anticipated.

Summary of Conclusions

1) A modification was surmised for conventional short-term dispersion models, such as the UNAMAP packaged PTMTP, to assess SO_2 levels around some Indiana power plants located in a rough terrain.

2) The alteration consisted simply of an artificial lowering of the hourly stability class by one when an appropriate combination of topography effects and meteorological patterns occurred. A suitable algorithm could be easily incorporated within the PTMTP model.

3) Projections based on decreased hourly stability were much closer to actually sampled SO_2 levels than conventional stability predictions.

4) Incorporation of similar procedures is suggested for any modeling scheme where strong mechanical turbulence due to surface friction is likely to occur.

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SEVERITY OF STATIONARY AIR POLLUTION SOURCES - A SIMULATION APPROACH

E. C. Eimutis, B. J. Holmes, L. B. Mote

Monsanto Research Corporation
Dayton, Ohio 45407

Abstract

A measure of specific point source air pollution severity has been defined as the ratio of its ground level concentration contribution of a given species relative to some potentially hazardous concentration of that species. For well-documented source types, e.g. coal-fired steam electric utilities, it is possible to analyze the severity on a plant-by-plant basis and to examine the severity frequency distribution deterministically. For many other source types, e.g. industrial/commercial boilers, cotton gins, asphalt batch plants, solvent evaporation, etc., the points of emission number in the thousands and in some cases in the hundred thousands. These source types require a statistical approach. We present a Monte Carlo simulation technique together with efficient algorithms for fitting the inverse Weibull, Gamma, normal, and log-normal cumulative density functions. Using coal-fired steam electric utilities as an example, we show a significant correlation between deterministic and simulated severity results.

Source Severity

The air pollution severity, S, of a given source should in some way be proportional to the degree of potential hazard it imposes upon individuals in its environment. The relative hazard, H, from a specific emission can be defined as being directly proportional to the delivered dose, the probability of dose delivery, and number of people who would receive it, and inversely proportional to the toxicity of the material as follows:

$$S \propto H \propto \frac{NP\Psi}{LD_{50}} \qquad (1)$$

where S = source severity
H = relative hazard
N = number of persons
LD_{50} = lethal dose for 50% of the people exposed
P = probability of dose delivery
Ψ = delivered dose = $B \cdot R' \cdot \int \chi(t)dt$
B = average breathing rate
R' = lung retention factor
$\chi(t)$ = concentration time history

The source severity is herein, defined as the ratio of the dose of a pollutant delivered to a population, relative to some potentially hazardous dose. Since LD_{50} data are not available for human beings, another measure of potentially hazardous dosage was used.

The potentially hazardous dose for a given pollutant from a specific point source in a given region is defined as follows:

$$\Psi_F = NBR' \int_{t_1}^{t_2} TLV(t)\ K\ dt \qquad (2)$$

where Ψ_F = potentially hazardous dose, g
N = population exposed to a specific source, persons
B = average breathing rate, m^3/s-person
R' = lung retention factor for the pollutant of interest (dimensionless factor, $0<R'<1$)
K = safety factor = $\frac{8}{24}\ \frac{1}{100}$
t = time
t_1 = start time, s
t_2 = finish time, s
TLV® = threshold limit value, g/m^3

The total time of interest, T, is defined as:

$$T = t_2 - t_1 \qquad (3)$$

Similarly, a hazard potential factor, F, is defined as:

$$F = TLV \cdot K \qquad (4)$$

Since TLV is a constant,

$$\Psi_F = N \cdot B \cdot R' \cdot T \cdot F \qquad (5)$$

The actual pollutant dose delivered, Ψ_A, from a given point source can be calculated as follows:

$$\Psi_A = N \cdot B \cdot R' \int_{t_1}^{t_2} \chi(t)\ dt \qquad (6)$$

where $\chi(t)$ = the actual ground level concentration time history of a pollutant of interest emitted by a specific point source, g/m^3

The value of $\chi(t)$ is very difficult to obtain and was therefore approximated by an average value, $\bar{\chi}$. The total actual dose delivered for a specific pollutant from a specific source is then:

$$\Psi_A = N \cdot B \cdot R' \cdot T \cdot \bar{\chi} \qquad (7)$$

Since our measure of source severity was defined as the ratio of the two dosages, then:

$$S = \frac{\Psi_A}{\Psi_F} = \frac{N \cdot B \cdot R' \cdot T \cdot \bar{\chi}}{N \cdot B \cdot R' \cdot T \cdot F} \qquad (8)$$

or

$$S = \frac{\bar{\chi}}{F} \qquad (9)$$

Simulation Methodology

In many statistical analyses of data, it is frequently desired to consider a random variable which is a function of other random variables. An example pertinent to air pollution studies is given by the severity equations for ground-level concentrations of air pollutants.[1] For example, the severity equation for SO_2 emissions from the stacks of coal-fired electric utility plants is given by:

$$S = \frac{50Q}{h^2} \qquad (10)$$

where Q = emission rate, g/s
h = emission height, m

The emission rate can be calculated from:

$$Q = (CC)(E)(\%\ \text{sulfur})(K_1) \qquad (11)$$

where CC = coal consumed, g/yr
E = emission factor = $\dfrac{0.019\ \text{g}\ SO_2(1\%\ \text{sulfur coal})}{\text{g of coal consumed}}$
% sulfur = percent of sulfur in the coal
K_1 = 3.171×10^{-8} (to convert g/yr to g/s)

or

$$S = \frac{(K_2)(CC)(\%\ \text{sulfur})}{h^2} \qquad (12)$$

where $K_2 = 3 \times 10^{-9}$

Next, consider a general setting where the random variable z is a function of the random variables $x_1, \ldots, x_n$ given by $z = f(x_1, \ldots, x_n)$ for some function f. Suppose the actual distributions of the input random variables $x_1, \ldots, x_n$ are known including their probability density functions (p.d.f.) and the corresponding cumulative distribution functions (c.d.f.). Then it seems reasonable to assume that the distribution of the random z can be obtained. In a sense this is true in that integral formulae have been developed which give the probability density function and the cumulative distribution function for z as a function of the same functions for the x_i.[2] These formulae, however, are complex even for the case of the simple sum, difference, product, or quotient of two random variables. Also, even if the integrals are successfully evaluated, the resulting probability density function for z will in general not be exactly one of the standard distributions and as a result may be difficult to handle. There are certain special cases in which the resulting p.d.f. will be known. In these instances, the analytical approach to finding z explicitly is by far the best approach. In other instances certain simplifying assumptions about the distribution of z can be made provided certain things are true about the coefficient of variability or equivalently the coefficient of skewness of the input variables. However, in cases where there are more than two input variables or there is considerable skewness exhibited by the variables or the function f becomes complicated, then the strict analytical approach to finding the distribution of z explicitly will in general not be applicable.

Sometimes it is desired to find information on the distribution of z when some things are known about the distribution of the input variables $x_1, \ldots, x_n$. Since the general approach of finding the explicit distribution function for z is not possible, "many" values of z may be calculated for explicit values of the input variables $x_1, \ldots, x_n$ and these values may be used to estimate (rather closely if enough values of z are known) such things as the mean, standard deviation, etc., for z. This approach is called the deterministic approach because in this technique it is possible to determine explicit values for z from explicit values of the input variables $x_1, \ldots, x_n$.

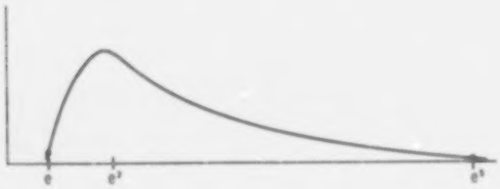
Consider the situation when either no explicit values of the input variable are available from which values of z can be calculated or the number of such values is too small to permit calculation of enough values of z to determine useful information regarding its distribution. In this situation we use a computer simulation to obtain values for z. For example, instead of knowing many values for the input variables $x_1, \ldots, x_n$, only limited information may be available, such as an estimate of the mean and possibly the range and symmetry or skewness properties. In this case, the input variables are fitted to some theoretical distribution and the small amount of available information about the variables is used to determine the parameters of the distributions. A computer is then used to sample from each input variable's distribution function and to subsequently use these data to calculate values of z from which the mean, standard deviation, etc., can be estimated and frequency histograms and cumulative distribution plots for z can be prepared. Some of the techniques and procedures used in such a computer simulation are described below.

The equation for the severity (equation 12) of ground-level concentrations of SO_2 emissions from the stacks of coal-fired electric utilities will be used to illustrate the methodology utilized in the simulation approach.

When all of the input random variables are independent random variables, the methodology is relatively simple. A large sample (e.g., of size n) is drawn from the distribution of each of the input variables. These data are then used one by one to calculate n values of S. From these n values of S, the mean, standard deviation, etc., can be calculated and a frequency histogram and cumulative distribution can be plotted.

Some comments are in order regarding the method by which samples are drawn from the distribution of the input variables. First, it should be noted that the input variables are restricted to one of four types of continuous distributions: the Weibull, Normal, Gamma, or Log-normal distribution. The type of each input variable and the corresponding parameters for its distribution function must thus be specified. The method of obtaining the "best" type for each variable and the corresponding parameters is described in another publication.[1] It is necessary to have a random sample of data points for the input variable in order to be able to fit it to the proper distribution. However, certain situations may arise when that much information about the input variable is not available. For example, two extreme points on the distribution and either the mean or mode may be known, or some information may be available to determine whether the distribution is symmetric or skewed. In such situations where the goodness-of-fit program is inoperable, it may still be possible to fit the variable to one of the four distributions above and to obtain its parameters.

As a demonstration of the above procedure, consider the following example. Suppose that for an input variable, x, it is known with 95% confidence that the values of x will be between e and e^5 (where e = 2.7..). Suppose also that the mode of the distribution is known to between e and e^2 and that the mean is approximately equal to e^3. These points then indicate that x is a rather heavily skewed right distribution. The graph for the p.d.f. of x may resemble the one shown below:



Since it is known that the 0.025 point on the cumulative graph is approximately equal to e and the 0.975 point is approximately equal to e^5, this information can be used alone to calculate A and B in a Weibull fit. Thus, one finds that A = 1.25 and B = 7.29×10^{-3}. These values of A and B yield a theoretical mean μ = 47.7 which is larger than the estimated e^3 value for the mean. The theoretical mode is 14.2 which again is larger than the estimated mode. Thus, the Weibull fit could be used as an approximation to the "true" distribution of x.

Another way of obtaining a distribution for x is to assume that it is log-normally distributed since the Log-normal distribution is a right-skewed distribution. If x is assumed to be a Log-normal distribution, then log x must be Normal. Hence, by taking the logarithm of the 0.025 point and 0.975 point of x, the same points on the cumulative graph of log x are obtained which were assumed to be Normal. These points are 1 and 5, respectively. Thus, the mean μ of log x should be taken to be 3 and, since 1 and 5 are the 0.025 and 0.975 points, respectively, it is found that σ = 1.2. The values μ = 3 and σ = 1.2 can thus be used as parameters to sample from the Normal for values of log x. By taking antilogarithms of the sample, a sample for x can be obtained.

In view of the above discussion, it is evident that several avenues are available for obtaining a distribution to fit the given data or information about each input variable. The simulation program (for the case of independent input variables) simply takes the parameters for the given type of distribution for an input variable and samples from this distribution to obtain a random sample for that input variable.

Example of Use of Simulation Approach with Coal-Fired Electric Utilities

In order to obtain an indication of how well the simulation procedure approximates the "true" population, SO_2 emissions from the stacks of coal-fired electric utilities were examined. Data were available on % sulfur, CC, and h for 224 power plants in the United States. This was considered to be the total population which was to be simulated by using only a small number (24) of plants in order to obtain information about the distributions of % sulfur, CC, and h.

To obtain a "random" sample, the first 24 plants on the list were selected. % sulfur, CC, and h for these 24 plants was then fitted to the four distributions considered in the simulation program. The distributions were then selected which appeared to fit the data better on an overall basis considering the SE, χ^2-value, actual class interval comparisons, and coefficient of skewness and measure of kurtosis calculations. For % sulfur, the Weibull Maximum Likelihood Fit was selected and clipped at the 5% and 99% points. Also, h was found not to be independent of CC. Hence, it was decided to treat h as a dependent variable correlated with the independent variable CC by using the raw data on the 24 plants to obtain R. The coefficient of skewness indicated that h was not normal but skewed to the right. Furthermore, the coefficient of skewness and measure of kurtosis for log h indicated "near-normality." Hence, it was decided to use the Log-normal distribution for h.

Using equation 12 for S, the data, as indicated above, are entered into the simulation program and 5000 values were calculated for S. Subsequently, the mean, standard deviation, maximum value, and minimum value were calculated. A deterministic calculation of these values was performed for all 224 plants in the population and the results are compiled in the table below:

Table 2 RESULTS OF DETERMINISTIC CALCULATIONS

Parameter	Simulated value	Deterministic value
Mean	9.25	8.9
Standard deviation	12.5	12.4
Maximum value	154.5	136.0
Minimum value	0.[illegible]8	0.36

Frequency histograms and cumulative frequency plots were also drawn for both the simulated values and the deterministic values of S and these are shown in Figures 1 through 4.

The large-sample t-test was performed to determine whether there was a significant difference in the simulated and deterministic mean values obtained above. The test, as might be expected, showed no significance in the difference at the 0.01 or 0.05 levels. Furthermore, the F test for significant difference in the variances was also negative, indicating no significant difference.

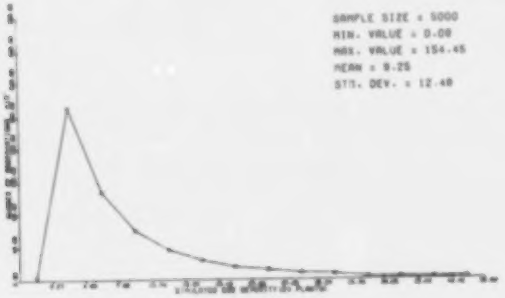


Figure 1. Frequency histogram for the severity of SO_2 emissions from coal-fired electric utilities using the simulation method.

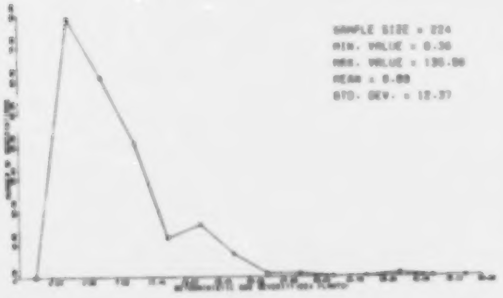


Figure 2. Frequency histogram for the severity of SO_2 emissions from coal-fired electric utilities using the deterministic method.

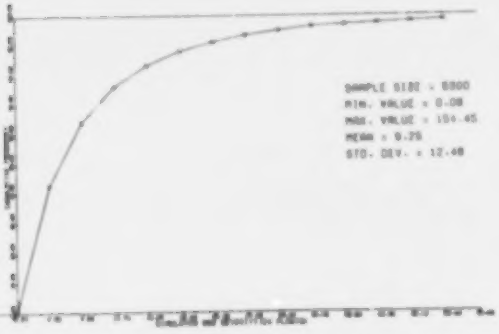


Figure 3. Cumulative frequency for the severity of SO_2 emissions from coal-fired electric utilities using the simulation method.

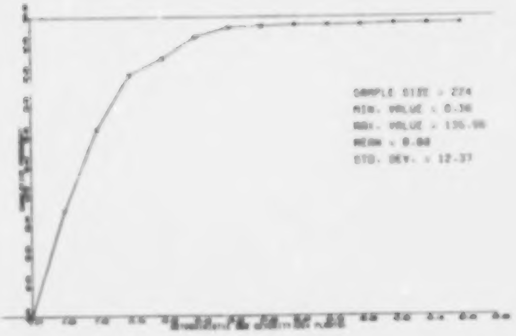


Figure 4. Cumulative frequency for the severity of SO_2 emissions from coal-fired electric utilities using the deterministic method.

Acknowledgments

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ATMOSPHERIC POLLUTANT DISPERSION USING SECOND-ORDER CLOSURE MODELING OF THE TURBULENCE[†]

W. S. Lewellen and M. Teske
Aeronautical Research Associates of Princeton, Inc.
Princeton, New Jersey

Abstract

A method is described for calculating turbulent diffusion of plumes in the planetary boundary layer based on Donaldson's second-order closure approach to turbulent flows. The method calls for solving dynamic, partial differential equations for the species flux, variance, and its mean concentration, as well as the second-order turbulent velocity and temperature correlations to determine the turbulence in the ambient atmospheric boundary layer in which the plume is embedded. The parameters governing dispersion in the planetary boundary layer are identified and discussed. Results from a sample calculation of dispersion in a free convection layer are compared with laboratory observations.

1. Introduction

A valid estimate of turbulent diffusion in the atmospheric boundary layer is required to determine the impact of a pollutant release on the air quality at some distance from the point of release. Our purpose here is to review and present some results from a model based on solving a specific dynamic differential equation for the turbulent flux of species. This approach, based on second-order closure of the ensemble-averaged moments of the fluctuating variables, is currently being studied by a number of investigators for computing turbulence in the atmosphere.[1-11] We review the essence of the model in the next section. The parameters identified by this model as governing the dispersion of a neutrally buoyant, nonreactive species in the planetary boundary layer are presented in Section 3. A sample calculation is compared with results from a laboratory simulation of dispersion in a free convection layer in Section 4.

2. Model Equations

We take as our starting point the ensemble-averaged, Eulerian equation of mass continuity for the species concentration C

$$\frac{\partial C}{\partial t} + \frac{\partial(U_i C + \overline{u_i c})}{\partial x_i} = S + D\frac{\partial^2 C}{\partial x_i^2} \qquad (1)$$

This equation is exact but undetermined even if the velocity U_i is known because of the presence of the additional variable $\overline{u_i c}$. By taking moments of the instantaneous variables and averaging, we can generate an exact equation for the species flux $\overline{u_i c}$.[2] This exact equation introduces variables other than second-order correlations and thus leaves the system of equations undetermined. The task of second-order closure is to model these terms as functions of the second-order correlations and mean flow variables.

Our philosophy has been to choose the simplest models that have proper tensor symmetry, dimensionalization, and the desired physical properties. The modeled form of the species flux equation may be written for high Reynolds numbers as

$$\frac{\partial\overline{u_i c}}{\partial t} + U_j\frac{\partial\overline{u_i c}}{\partial x_j} = -\overline{u_i u_j}\frac{\partial C}{\partial x_j} - \overline{u_j c}\frac{\partial U_i}{\partial x_j} + \frac{g_i\overline{c\theta}}{\theta_o} + 0.3\frac{\partial}{\partial x_j}\left(q_p\Lambda_p\frac{\partial\overline{u_i c}}{\partial x_j}\right) - \frac{3q_p\overline{u_i c}}{4\Lambda_p} \qquad (2)$$

We do not expect that the last two modeled terms in Eq. (2) used to replace the complex terms of the exact equation will faithfully represent all of the information present. However, for most problems, we are interested in only a small part of the information contained in the complete turbulent spectrum. We believe that the two modeled terms provide at least the minimum amount of desired information needed to close the system at the second order. The first modeled term introduces diffusion to prevent excessive gradients in the species flux. The other modeled term, a tendency-towards-isotropy term, introduces the required feedback which permits the flux to reach an equilibrium level even in the presence of large production contributed by the first three exact terms on the right-hand side of Eq. (2).

The effect of stability on diffusion comes into Eq. (2) in two ways: through the influence of stability on the velocity fluctuations[2] and through the buoyant term appearing directly in Eq. (2). This term is not a result of our closure modeling but arises directly from the buoyant term in the momentum equation. However, modeled terms must appear in the equation derived for $\overline{c\theta}$. If these are treated in a similar fashion to those in Eq. (2), the equation for $\overline{c\theta}$ may be written as

$$\frac{\partial\overline{c\theta}}{\partial t} + U_j\frac{\partial\overline{c\theta}}{\partial x_j} = -\overline{u_j\theta}\frac{\partial C}{\partial x_j} - \overline{u_j c}\frac{\partial\Theta}{\partial x_j} + 0.3\frac{\partial}{\partial x_j}\left(q_p\Lambda_p\frac{\partial\overline{c\theta}}{\partial x_j}\right) - \frac{0.45q_p\overline{c\theta}}{\Lambda_p} \qquad (3)$$

With the velocity and temperature fields specified, Eqs. (1), (2) and (3) form a complete set for the determination of C. The velocity and length scales, q_p and Λ_p, appearing in Eqs. (2) and (3), are appropriately related to the companion scales q

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and Λ of the ambient turbulent field. The mean velocity, temperature, and second-order velocity and temperature fluctuations may be obtained from field observations or calculated from similarly modeled equations.[2,9,10] As long as we are dealing with a nonreactive, neutrally buoyant species, the two sets need not be coupled together.

3. Governing Parameters

A solution to the dispersion equations, Eqs. (1-3), for a neutrally buoyant, nonreactive species requires specification of the velocity U_1 ; temperature, Θ ; Reynolds stress, $\overline{u_1 u_j}$; heat flux, $\overline{u_1 \theta}$; turbulent scale, Λ ; and source S , as functions of time and space. Although one may argue with the details of our modeling, it appears unlikely that a more accurate model would require less information. Thus, very detailed measurements of turbulence are required if one attempts to predict dispersion on the basis of measured wind and turbulence fields alone. Measurement of the average wind speed and direction plus an estimate of the stability class of the turbulence are unlikely to provide sufficiently accurate data.

It is naturally desirable to parameterize this dependence with as few a number of parameters as possible. The critical parameters may be deduced by examining the equations governing the ambient turbulence in the planetary boundary layer.[10]

A. Surface Layer Parameterization

Within the surface layer, when the equilibration time Λ/q of the turbulence is small in comparison to flow times over changes in surface features, a few direct parameters will suffice. Estimates of the surface shear stress, u_* , surface heat flux, θ_* , and the effective surface roughness, z_o , are adequate to specify the wind, temperature, and turbulence fields completely through the Monin-Obukhov similarity functions. These empirically correlated functions may in fact be predicted from our modeled turbulence equations in the limit of stationary, unidirectional flow with u_* and θ_* held fixed, while the other variables are allowed to be functions of the vertical coordinate alone.[4] For this to be true, it is necessary to have $(U_1 \Lambda_p/q_p(\ ))\partial(\ )/\partial x_1 \ll 1$. This same restriction may be applied to the species flux equation, Eq. (2). If we also neglect the diffusion terms, which should be small in the lower portions of the surface layer where $\Lambda_p = \Lambda = 0.65z$, and $q_p = q$, then Eq. (3) may be used to eliminate $\overline{c\theta}$, and an algebraic expression for $\overline{wc}$ obtained. Thus,

$$\overline{wc} = -\left[\frac{\left(\frac{4\overline{ww}\Lambda}{3q} + \frac{g}{\Theta_o}\frac{\Lambda^2\overline{w\theta}}{0.34q^2}\right)}{\left(1 + \frac{g}{\Theta_o}\frac{\Lambda^2}{0.34q^2}\frac{\partial\Theta}{\partial z}\right)}\right]\frac{\partial C}{\partial z} \qquad (4)$$

The bracketed quantity in Eq. (4) defines an effective eddy viscosity K which is a function only of u_* , z and L . This surface-layer K is plotted in Fig. 1 normalized by its neutral value of $0.52u_*z$. It is a strong function of z/L .

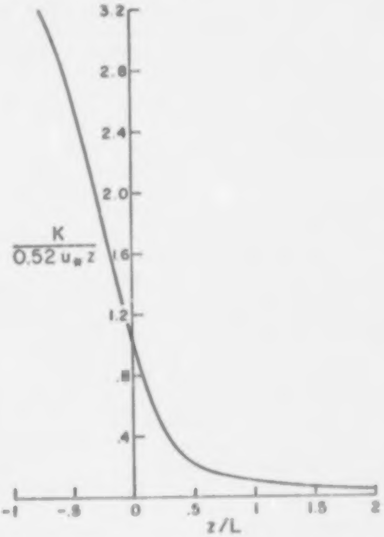

Fig. 1. Effective turbulent diffusion coefficient K as a function of height and Monin-Obukhov length L in the surface layer as predicted by the superequilibrium limit of our turbulent model.

The downstream vertical dispersion of a plume from its source depends on the wind distribution as well as K . This observation introduces a dependence on z_o in addition to u_* and L . Under neutral conditions, the surface layer extends to approximately 100m; under very stable conditions its extent may be reduced to only 20m. Under unstable conditions the height of the surface layer depends upon the height of the inversion layer at the top of the planetary boundary layer. Surface layer approximations are valid in this case for $z/z_i < 0.1$. In no case, however, is the surface layer approximation valid above an altitude of a few hundred meters.

The only difficulty with dispersion in the surface layer is the prediction of the horizontal dispersion. The conditions necessary for the horizontal wind variance to obey Monin-Obukhov similarity are much more strenuous than those for the vertical variance. This fact is reflected in the large scatter observed in the reported measured values of the horizontal wind variance in the surface layer.[11] Theoretically, the cause appears to be the low frequency lateral velocity fluctuations forced by inhomogeneities in terrain or mesoscale meteorological phenomena. These low frequency flucuations have a much larger time constant associated with their decay. Thus, the flow conditions must be steady and spatially homogeneous on a much larger scale for the horizontal wind variance to satisfy in detail the surface layer approximation necessary for Monin-Obukhov similarity to hold.

B. Parameterization in the Ideal Planetary Boundary Layer

Above the surface layer region the parameterization of dispersion becomes much more complicated. Not only are several additional parameters introduced, but the time required for the flow to reach an equilibrium state is greatly increased. The characteristic time for the neutral planetary boundary layer is the reciprocal of the Coriolis parameter f (approximately 3 hours at mid-latitudes). In practice neutral conditions rarely exist long enough for the steady state, neutral layer to be achieved. Rather, the surface heat flux forces a continuing evolution of the boundary layer above it. This evolution as a function of time for a typical summer day in the Midwest , as computed by our model, has been given previously.[7,10] Similar calculations using different versions of the closure model have been made by Mellor and Yamada.[6,11]

At sunrise an unstable surface layer begins to grow, developing into a deep mixing layer with high turbulence by afternoon. The height of the unstable mixed layer then continues to increase slowly until sunset. Shortly after sunset a stable layer with a temperature inversion develops at the surface. This surface inversion layer increases in depth during the nocturnal hours while the upper level inversion slowly decreases in altitude. This development leaves a mixed layer of decaying turbulence trapped between the two inversion layers until the unstable surface layer breaks through the low-level inversion the next morning to re-energize this region. The turbulence distribution across the entire boundary layer at any particular time of day may only be crudely represented by a single stability parameter.

Because of the slow growth of the nocturnal, low-level inversion during the early morning hours, it is possible to parameterize approximately the distribution below this altitude as a function of a single stability parameter (such as a Richardson number) and a Rossby number parameter to indicate the relative importance of rotation. We may also approximate the strongly unstable distributions in terms of the characteristic velocity w_* appropriate for free convection. Our model prediction for the vertical variance in this limiting similarity form compares quite well with laboratory simulations.[9] Away from this limiting case, two parameters, one measuring the stability and one measuring the height of the inversion layer, are required to specify the distributions even under quasi-steady conditions. These two parameters may be taken as a Richardson number Ri and as the ratio of the inversion height to the Monin-Obukov length z_i/L . The relative influence of Rossby number and Richardson number on the profiles of the quasi-steady wind and vertical velocity variance are shown in Fig. 2. Several observations are: (1) for equal Ro the neutral or stable boundary layer becomes thicker as the distance from the equator and/or the geostrophic wind increases; (2) the dimensionless height of the boundary layer is reduced as Ro increases; (3) the crosswind, perpendicular to the geostrophic wind, increases as Ro increases; (4) increasing Ri also increases the crosswind component and decreases the boundary layer thickness; (5) the only significant shift in the direction of the wind with altitude for the unstable profiles is in the vicinity of the upper level inversion.

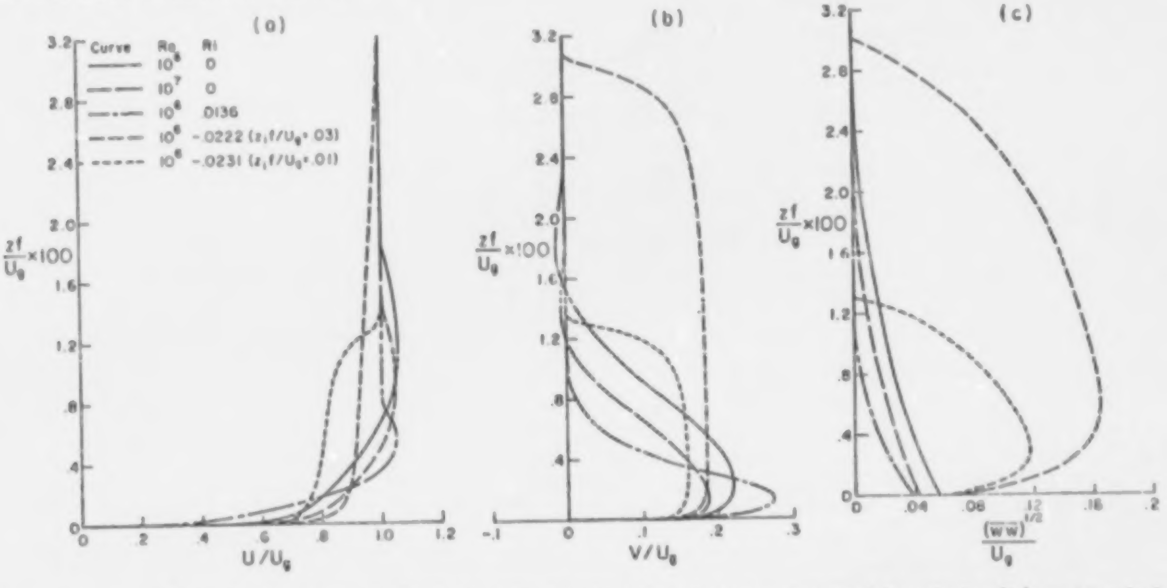

Fig. 2. Profiles for (a) mean wind in the direction of the geostrophic wind, (b) mean wind in the direction normal to the geostrophic wind, (c) vertical velocity variance, for various values of $Ro = U_g/z_o f$ and Ri , the bulk Richardson number based on the velocity and temperature differences between the surface and 10m height. The height may be read directly in Km for $U_g = 10 m/sec$ and $f = 10^{-4} sec^{-1}$.

These limiting parameterizable cases probably occur more often than the neutral, steady-state profiles, but still represent the exception rather than the rule. Even in an ideal diurnal variation case, the parameterization would represent somewhat less than half of the altitude-time domain, since it does not account for the mixed layer between the two inversion layers between sunset and noon the next day. When the diurnal surface heat flux variation is significantly reduced in the presence of a relatively strong stable lapse rate, the altitude of the top inversion layer is drastically reduced and the domain over which this parameterization is valid correspondingly decreases.[13]

At least two other physical mechanisms reduce the domain over which the previously presented parameterization is valid: baroclinicity and radiation flux divergence. Both of these influences are frequently present in the planetary boundary layer. Not only do they serve to increase the number of parameters governing the flow, but they introduce additional dynamics and reduce the time over which the quasi-steady parameterization is valid. Results for some assumed time variations of these two influences as calculated by our model have been presented in ref. 13. Even when influences of nonhomogeneous terrain are eliminated, the characterization of the wind and turbulence distributions in the planetary boundary layer in terms of two or three parameters is necessarily rough and at time highly erroneous. We believe much better results for a valid prediction of the distributions at any given time may be found by tracking the time variation of the forcing boundary conditions for at least twelve hours prior to the desired observation time.

C. Additional Dynamics Introduced by Diffusion Equations

When the wind and turbulence fields are known, the additional parameters necessary to determine the dispersal of a neutrally buoyant, nonreactive species are those necessary to characterize the source S. Whenever the characteristic time scale of the turbulent mixing is much less than any time scale t_s associated with S, the left-hand side of Eq. (2) may be neglected and a superequilibrium (or K) theory should be approximately valid. In the surface layer this reduction would lead to Eq. (4) for K. Although this approximation will not be valid for pollutant sources with sufficient spatial inhomogeneities, it should be useful in many cases and, in fact, probably forms the basis of the limited success of Gaussian plume models parameterized for different stability classes.

It is easy to think of many cases where Λ/q is no longer much smaller than t_s. Two common examples are when $\Lambda_p \ll \Lambda$, or when the plume scale divided by the crosswind velocity is less than or of the same order as Λ/q. In such cases K theory may lead to considerable error. In general, reliable diffusion models must be able to compute $\overline{u_1 c}$ accurately whether or not the time rate of change of $\overline{u_1 c}$ (or the advection of $\overline{u_1 c}$) is significant. We believe Eq. (2) has this capability. Results of sample calculations for both line and point source releases have been presented elsewhere.[10,14] Space limits us to one example here.

4. Sample Calculation for Free Convection

Figure 3 presents the results of a sample model calculation for dispersion in a free convection mixed layer. Deardorff and Willis[15,16] simulated dispersion in the atmospheric mixed layer by releasing a large number of small, neutrally buoyant particles as an instantaneous line source into the bottom of a water convection tank. They interpret their results in terms of a continuous point source release into a uniform wind. Initial comparisons of our predictions with their observations for both the species dispersal and turbulence field have been made.[10,14] Here we will take advantage of their most recent published results[16] to update this comparison.

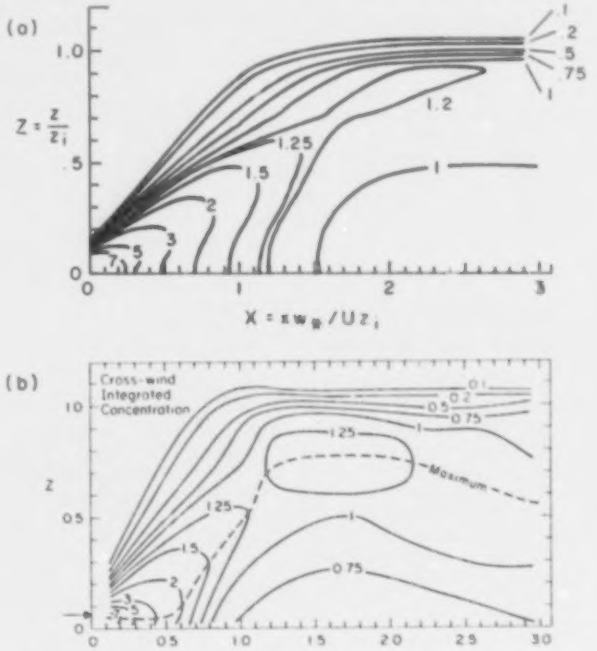

Fig. 3. Isopleths of the crosswind integrated concentration, $\overline{C}^y$, as a function of downstream distance and height when a continuous point source is released into an unstable mixed layer. (a) Model predictions; (b) Laboratory observations of Deardorff and Willis.[16]

We begin our calculations with a Gaussian plume distribution with $\sigma_y = \sigma_z = 0.006 z_i$, since our model can not actually start with a point release. A uniform wind is applied and the calculation marches in x, the direction of the wind, to follow the plume development. We plot the variation of the normalized crosswind integral of the concentration

$$\overline{C}^y = \int_{-\infty}^{+\infty} \frac{CUz_1}{S}\, dy \qquad (5)$$

In the completely mixed layer, approached as $x \to \infty$, $\overline{C}^y = 1$ for all z. In the early development of the plume, both the observations and the predictions show the local maximum in concentration rising above the level of initial source, $z_s = 0.067z_1$. Willis and Deardorff show that this effect would correspond to a negative K over much of the spatial domain if one attempted to predict this by K theory alone. In our model it is a direct result of the buoyant forcing term in Eq. (2).

The greatest discrepancy between the predictions and the observations occurs in the upper portions of the plume during the early development and at the surface near $X = 1$. The discrepancy at the upper edge of the plume may be partially due to the low Reynolds number of the experiment ($\simeq 1730$ when based on q and z_1) while our model run was made for much higher Re ($\simeq 10^7$) to more nearly simulate atmospheric conditions, but probably reflects some error in our turbulent scale as the inversion layer is approached. The higher rise of the plume as well as a stronger horizontal dispersion of the plume at altitude allows the observed surface concentration to be lower than that predicted. The general character of the dispersion is quite favorably predicted, especially considering the fact that no empirical information from this particular experiment has been used in determining the model.

5. Concluding Remarks

Our model is currently capable of making calculations for individual, neutrally buoyant, nonreactive plumes. A three-dimensional source release may be followed if the wind and turbulent fields are assumed stationary over the characteristic time required for the development of the plume. For a two-dimensional source release this stationarity requirement may be relaxed, but the wind field must be independent of the third dimension. Steps are now underway to incorporate the capability to compute a buoyant plume with internally generated turbulence. Some refinements in the modeled terms and coefficients should be expected as more comparisons with reliable measurements are made and as fundamental theoretical work proceeds. However, comparison of the results of the current model with experimental observations demonstrates that it is a valid tool for studying the sensitivity of dispersion to different time and space variations of the boundary conditions on the planetary boundary layer.

The model shows that quasi-steady parameterization is valid within the surface layer, and in some limited regions of the physically realizable time-altitude domain of the planetary boundary layer; but, solution of the species flux equation appears to be the way to deal more accurately with the dispersal problem in general.

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POINT SOURCE TRANSPORT MODEL WITH A SIMPLE DIFFUSION CALCULATION FOR ST. LOUIS

Terry L. Clark*

Robert Eskridge*

Meteorology and Assessment Division
Environmental Sciences and Research Laboratory
Environmental Research Center
Research Triangle Park, N.C. 27711

Abstract

The transport of an inert gaseous contaminant in St. Louis is modelled by a numerical method. The numerical model calculates, from a wind field, a two-dimensional field of streamfunction values characterizing the air flow. The wind field is objectively analyzed from 15-minute averaged RAPS (Regional Air Pollution Study) data using orthogonal functions. The streamfunction values are calculated from an elliptic equation solved by successive over-relaxation.

After assuming a non-divergent, two-dimensional flow, streamlines are analyzed from the streamfunction field. Trajectories are then computed by displacing puffs of a contaminant along a specified streamline. A simple diffusion calculation is included in the model to demonstrate one of its possible uses.

Measurements obtained from a SF_6 tracer study provide data with which the results of the transport model are compared. Six of the nine sets of measurements obtained along 3 highways in St. Louis during August 12-13, 1975 are considered.

Introduction

Accurate simulation of air pollution concentrations has been of interest for many years beginning with the works of Roberts.[1] He developed the basic plume formulas, which have been used for point source releases and other applications. Mathematical models based upon these and other formulations have been developed to simulate air pollution concentrations. In the last several years, urban-scale grid point models have been developed by Systems Applications Incorporated and IBM [2,3]. In addition, an urban-scale trajectory grid point model has been developed by Eschenroeder.[4]

The grid point models include variable winds, but because of limited resolution, are unable to be applied to single point-source cases. Gaussian plume models, on the other hand, are capable of calculating concentrations for single point sources, but do not account for variable wind velocities. A model with a high spatial resolution that employs wind fields varying over short periods of time would be useful on an urban-scale. Some practical uses of this type of model would include identifying areas affected by instantaneous releases from one or more point sources and supplying the transport mechanism for deposition studies.

The transport model described in this paper was developed to apply to instantaneous point-source emissions in the form of puffs. Wind and streamfunction fields, from which trajectories were calculated, were generated from 15-minute averaged data. The calculation of trajectories ensured a spatial resolution much better than the grid point models. Moreover, the selected averaging period reflected small-scale changes of the wind velocity, which theoretically, would enhance the quality of the trajectory calculations.

In this paper, the development of the transport model and results of six puff releases are described. The results were compared to an Atmospheric Tracer Study which involved continuous SF_6 releases. In order to demonstrate the usefulness of the transport model, a simple diffusion calculation was added. A more complex diffusion calculation can be substituted easily.

Data

A. Meteorological

The wind fields employed in this application of the transport model were analyzed from wind data measured from the Regional Air Pollution Study (RAPS) in St. Louis, Missouri during August of 1975. The Regional Air Monitoring Stations (RAMS) network consists of 25 sites, 21 of which are located within 26 km of downtown St. Louis (Fig. 1). Data from these 21 sites were considered for the wind analyses. The grid locations of two of these sites, namely 116 and 121, were relocated slightly so that they were located on the wind analysis grid. One-minute averages of wind speed and direction were obtained from continuous measurements atop a 10-meter tower at sites 108,110,114-118, and 121 and a 30-meter tower at the remaining sites. The height differences of the levels of measurements accounted for local obstructions to the air flow. After the data were validated, 15-minute averages were computed for each site for selected time periods.

B. Tracer Measurements

Measurements from the Atmospheric Tracer Study taken by the California Institute of Technology in August of 1975 were employed to compare the results of the trajectory and concentration computations.[5] In this study, continuous releases of SF_6 tracer were completed from one of three sites in St. Louis during five periods in August of 1975. The results of the model corresponding to the tracer study case for August 12-13 are discussed in this paper.

The SF_6 tracer was released, in this case, from a point 20 feet above the ground at Webster College (just to the southwest of St. Louis) from 8:40 P.M. until 3:00 A.M. at a rate of 6.2 gm sec^{-1}.

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* On assignment from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce

During this period, the sky was clear, the surface temperatures were in the lower 70's, and the winds were strong from the south-southwest.

Between 10:25 P.M. on August 12 and 2:26 A.M. on August 13, 9 automobile traverses were conducted along segments of 3 highways in St. Louis where the SF_6 plume was expected to pass. Throughout each traverse, a passenger in the automobiles took a grab sample in a 30 cm^3 plastic syringe every 0.1, 0.2, 0.3, 0.4, or 0.5 miles along the route. The interval depended upon both the distance from the point source and the steadiness of the wind.

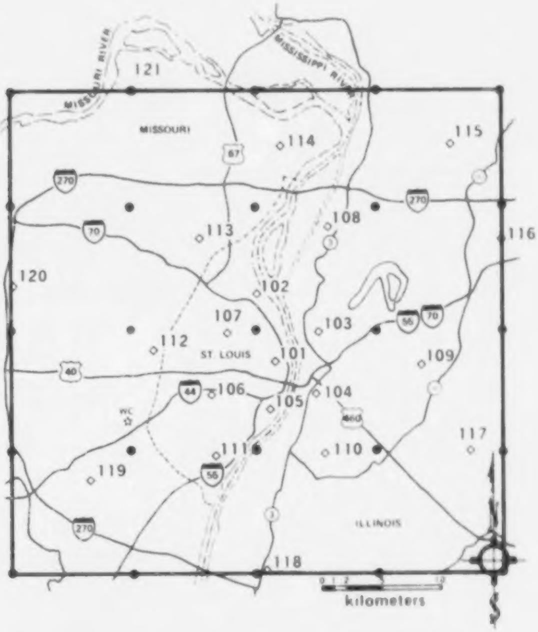

Fig. 1. The 40 x 40 km analysis grid and location of 21 of the 25 RAMS sites in St. Louis, Missouri. Every tenth grid point on the interior and every tenth grid point on the boundary are indicated. The "*" indicates the location of Webster College.

Wind Field Analysis

Meridional, zonal, and resultant wind fields were objectively analyzed on a 40 x 40 grid (Fig. 1) by a technique based upon a generalized orthogonal function approach developed by Jalickee and Rasmusson.[6] The technique prescribes a relationship between a set of M observations,

$$h_i \quad , \quad i = 1,2,\ldots\ldots,M$$

with space-time coordinates,

$$\phi\, i\,(x_i, y_i, z_i, t_i) \quad , \quad i = 1,2,\ldots\ldots,M$$

and a set of N base functions,

$$f_k \quad , \quad k = 1,2,\ldots\ldots,N$$

multiplied by a set of coefficients,

$$b_k \quad , \quad k = 1,2,\ldots\ldots,N$$

according to Eq. 1.

$$h_i = \sum_{k=1}^{N} b_k f_k(\phi_i) + z_i \qquad (1)$$

The term, z_i represents a random variable signifying noise in the observations.

The particular set of 15 base functions employed in the model were

$$1, x, xy, y, x^2, x^2y, x^2y^2, xy^2, y^2, x^3, x^3y, xy^3, y^3, x^4, y^4 .$$

The optimal set of coefficients was determined by minimizing the quantity

$$\left[h_i - \sum_{k=1}^{15} b_k f_k(\phi_i) \right]^2 \quad .$$

The resulting equation $(\sum_{k=1}^{15} b_k f_k)$ was employed to determine grid point values of the u - or v - components of the wind.

This objective analysis technique also produces a field of confidence values, associated with the u - or v - component wind fields. This served as a means to determine the quality of the analysis at a particular portion of the grid.

At first, the data from RAMS sites 101-121 served as the input to the objective analysis procedure. However, it was later discovered that the over-all analyses improved when the data from a few of the RAMS sites were omitted from the densely-instrumented center of the grid. The polynomial of degree four fitted the data especially well in the center of the grid when all the available data were employed. However, the values of the u - and v - components near the boundary were much larger than the values at the center of grid. After experimentation it was discovered that when sites 103 and 104 were omitted the analyses improved.

Moreover, it was discovered that the best results of the analyses were obtained when there were no attempts made to extrapolate beyond the data points. To prevent this from occurring, wind velocities were specified at the grid corners of the analysis fields. The velocities specified were identical to the velocities at the nearest data point to the corner. The data from RAMS site #115 was used for data at the upper right corner; #117 for the lower right; #119 for the lower left; and #121 for the upper left. Although the possibility of an error had been introduced, the resulting analyses were more agreeable with the data.

The quality of the analyses, naturally, was dependent upon the quality of the data sample. Unfortunately, wind data were either questionable or missing from 3 to 6 of the 19 RAMS sites considered in every analysis. Almost in every instance, wind data were lacking from sites adjacent to the tracer plumes in the tracer study and other key locations.

Parcel Trajectory Calculation

Trajectories of parcels generally have been calculated by averaging wind data or gridded wind values in the vicinity of the parcel (e.g., Heffter, et.al.).[7] For this reason, this type of approach can be referred to as a "local" approach. For the transport model, the trajectories were calculated from the entire wind field. Hence, a global approach was adopted.

After the wind fields were analyzed on the 40 x 40 grid, values of the streamfunction were calculated on a 20 x 20 grid of identical grid spacing which was a subset of the former. It was found that the analyses were more agreeable with the data when determined from a smaller grid. The values obtained at each grid point were dependent upon the total wind field, due to the iterative process employed. Isolines of the resulting streamfunction values represented streamlines for the case of two-dimensional, non-divergent flow.

Assuming this type of flow, the equation of continuity can be written as

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0. \tag{2}$$

The streamfunction, $\psi(x,y)$, can be defined by Eq. 3 and can be shown to satisfy the equation of continuity (Eq. 4).

$$\frac{\partial \psi}{\partial x} = v \text{ and } \frac{\partial \psi}{\partial y} = -u \tag{3}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = \frac{-\partial^2 \psi}{\partial x \partial y} + \frac{\partial^2 \psi}{\partial x \partial y} = 0 \tag{4}$$

By using the vertical component of the vorticity (Eq. 5), the streamfunction can be related to the wind field by Eq. 6. This form of the streamfunction equation was used in the model.

$$\zeta = \vec{k} \cdot \vec{\nabla} \times \vec{v} = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \tag{5}$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \zeta(x,y) \tag{6}$$

The first step in the streamfunction calculation consisted of the specification of ψ along the boundary. The streamfunction value at the bottom left corner (southwest corner) of the grid was defined to be zero. The remaining boundary values were calculated first along the bottom and right borders and then along the left and top borders using Eq. 3.

This procedure yielded two values of approximate magnitude at the top right corner, however; one from the right border ($\psi^r_{20,20}$) and one from the top border ($\psi^t_{20,20}$). As long as the signs of the two values were identical, an insignificant error was introduced when the arithmetic average of the two ($\bar{\psi}_{20,20}$) was assigned to the corner grid point. The reason for the condition that the signs be identical is explained later.

The border values of the streamfunction were forced to be greater than zero by adding to each border value, the absolute value of the smallest negative border value. This adjustment would not alter the streamline analysis since streamlines are lines of constant values of the streamfunction for two-dimensional, non-divergent flow. After this adjustment was executed, the streamfunction value at the bottom left corner was no longer zero.

In order to smooth false gradients near the top right corner of the grid due to the averaging process, the border values again were adjusted. The values along the bottom and right borders were multiplied by the factor

$$(\bar{\psi}_{20,20} \;/\; \psi^r_{20,20}).$$

Similarly, the values along the left and top borders were multiplied by a factor of

$$(\bar{\psi}_{20,20} \;/\; \psi^t_{20,20}).$$

These factors tended to be of the order of unity, while the streamfunction values tended to approximate 10^5. Therefore, the adjustment was a minor one. If the signs of these two factors were different, this adjustment procedure yielded a less accurate streamfunction analysis, since the sign of some border values would change and the others remain unchanged. This could introduce large changes in the orientation of the streamlines.

The second step involved the determination of the streamfunction values at the interior points of the grid. This was accomplished by the iteration of a four-point explicit form of the streamfunction equation (Eq. 7).

$$\psi_{ij} = \psi_{ij} + \frac{\alpha}{4}\Big\{\psi_{i-i,j} + \psi_{i,j+i} + \psi_{i+i,j} + \psi_{i,j-i} - 4\psi_{i,j} - \frac{\Delta h}{2}\Big(v_{i+i,j} - v_{i-i,j} - u_{i,j+i} + u_{i,j-1}\Big)\Big\}, \tag{7}$$

where Δh is the grid spacing and α is an over-relaxation factor employed to force the solution to converge more quickly. The optimal[8] value of the factor is the smaller root of Eq. 8.

$$\alpha^2 t^2 - 4\alpha + 1 = 0, \tag{8}$$

where $t = \cos\frac{\pi}{p} + \cos\frac{\pi}{q}$

and p and q are the number of grid points in the x and y direction, respectively.

The terms in Eq. 7 represent values of the streamfunction or wind components at the grid points specified by the subscripts. The value of the streamfunction at grid point (i,j) was dependent upon the values at (i,j) and the four nearest grid points from the previous iteration. Prior to the first iterative step, the values of the streamfunction were set to zero at the interior grid points. The streamline analysis resulting from the streamfunction calculation for the 15-minute period centered around 11:52 P.M. on August 12, 1975 is depicted in Fig. 2.

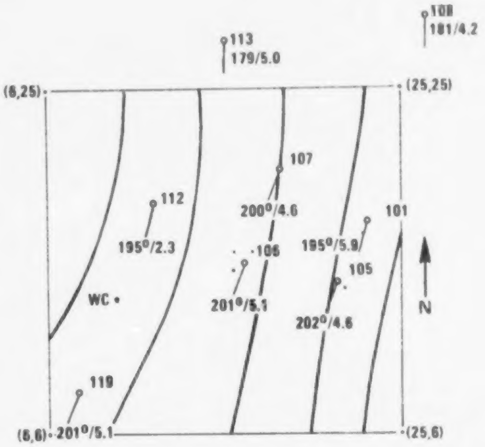

Figure 2. Depiction of the streamline analysis on the 20 x 20 streamfunction computational grid for the 15-minute period centered around 11:52 P.M. on August 12, 1975. The 15-minute-averaged wind velocities are indicated at the RAMS sites within and near the 20 x 20 grid.

After the grid point values of the streamfunction were calculated, the value of the streamfunction at the specified location of the parcel or puff was determined. This was accomplished by the use of a 16-point interpolation scheme developed by Gandin and Boltenkov.[9] This value identified the isoline or streamline the puff would follow during the ensuing 15-minute period.

Next, the equation of the particular streamline was determined. First, the points where the streamline intersected the borders of the 16 grid squares nearest the puff were identified. The identification was made possible by the use of an interpolation scheme employing finite differences (Eq. 9).

$$P(x) = f[x_0] + f[x_1,x_0](x-x_0) + f[x_2,x_1,x_0](x-x_0)(x-x_1) \qquad (9)$$

where x_0, x_1, and x_2 are x- coordinates on the grid. The y- coordinates of the points of intersection are calculated in a similar fashion.

The x- coordinate of the initial location of the puff (x_0) and the x- coordinates of the two nearest points of intersection downwind from the puff (x_1, x_2) were fitted by a quadratic polynomial, g(x), using finite differences (Eq. 9.). The puff was then displaced along the curve described by g(x) at a rate equal to an interpolated value of the wind speed for a period of 100 seconds. The final displacement position relative to the starting point was determined by using the arc length. Eq. 10 is the arc length formula used to calculate the puff displacement in the x direction. The formula to calculate the puff displacement in the y direction is similar.

$$D = \int_{x_0}^{x_f} (1 + g(x)^2)^{1/2}\, dx \;, \qquad (10)$$

where $g(x) = ax^2 + bx + c$.

The values of x_0 and D were known and x_f was determined by Newton's method. The value of x_f, which represented the displacement along the x- axis, was added to or subtracted from the position along the axis at the end of the 100-second period.

This process was repeated 8 more times using the same wind field. At the termination of 900 seconds (15 minutes), a new wind field was calculated based upon up-dated, 15-minute averaged winds. The puff was transported for an additional 15 minutes starting from the termination point of the previous period. This process ended when the position of the puff was beyond the area where the plume from the tracer study was sampled.

Concentration Calculation

The concentration of each puff was calculated at the end of each 100-second period. This was performed using a diffusion calculation based upon Eq. 11, which was derived by Roberts.[1]

$$\overline{c}(x,y,z) = \frac{Q}{8(\pi Kt)^{3/2}} \exp\left(\frac{-r^2}{4Kt}\right) \;, \qquad (11)$$

where Q is the initial generation of contaminant (gm); K is the diffusion coefficient (m^2 sec^{-1}); t represents the time after the release of the puff from the source (sec); and r is the distance from the center of the puff (m). From the tracer study, the emission rate of SF_6 was known. The value assigned to Q in Eq. 11 was the mass of SF_6 emitted during a one-minute period.

It was assumed that the diffusion coefficients along the x-, y-, and z- axes were equal to a constant coefficient, K. However, the method of determining the values of the coefficient was beyond the scope of this research. The treatment of the K- theory in existing models was examined instead. The pollution model constructed by IBM assumed a value of 500 m^2 sec^{-1}.[7] The planetary boundary layer model developed by Gerrity used values of K between 1 and 100 m^2 sec^{-1}.[10] In the transport model, a value of 10 was chosen for generally stable conditions and 100 m^2 sec^{-1} for generally unstable conditions.

Results and Conclusions

The results of the transport model for 6 of the 9 instrumented automobile traverses of the St. Louis tracer study during August 12 and 13, 1975 are presented in Figs. 3A-F. The puff positions are shown on the 40 x 40 km grid at the termination of every 15-minute period. In every case, the source point was located at Webster College (denoted by "WC") near the southwest corner of the grid. The shaded numbers indicate RAMS sites where data was omitted intentionally (#103 and #104 on the east side of St. Louis), or either missing or highly questionable. It is important to note that data were missing from several key sites throughout the periods.

The small bars along portions of highways #40, #70, and #270 represent segments of the roads where SF_6 tracer was measured via the traversing automobiles. The maximum measured concentrations of the SF_6 plumes are listed adjacent to each figure. This value might not equal the actual maximum concentration, since grab samples were taken at prescribed intervals along the routes.

Fig. 3A indicates that the model transported the puff released at 12:30 A.M. across highway #40 at a point 1.5 km east of the area where the plume was detected. At this point, the puff was 5 km downwind from Webster College. The calculated concentration at the surface directly beneath the center of the puff was 841 ppt (parts per trillion). This is 30% of the maximum concentration measured at this time.

Fig. 3B shows that the puff released at midnight traversed highway #70 at approximately 1:00 A.M. The point of intersection agrees with the measurements. At this time, the puff was 14 km from the source. The calculated concentration was 220 ppt or 91% of the maximum concentration measured there.

Fig. 3C indicates that the puff released at 11:45 P.M. on August 12 traversed highway #270 at approximately 1:15 A.M. on August 13. The point of intersection also agrees with the tracer study data. The puff at this time was approximately 20 km from the source point. The concentration calculated as the puff crossed the highway was 122 ppt, which is 67% of the maximum concentration measured.

Fig. 3D indicates that the puff released at 1:45 A.M. crossed highway #40 at a point less than 1 km from the section of the highway where the tracer plume was detected. At this point, the puff was 5 km from the source point. The calculated concentration at this time was 841 ppt or 43% of the maximum concentration measured.

Fig. 3E shows that the puff released at 1:00 A.M. crossed highway #70 at a point where the tracer plume was detected. The puff at this time was approximately 14 km from the source. The concentration calculated was 286 ppt or 47% of the maximum concentration measured.

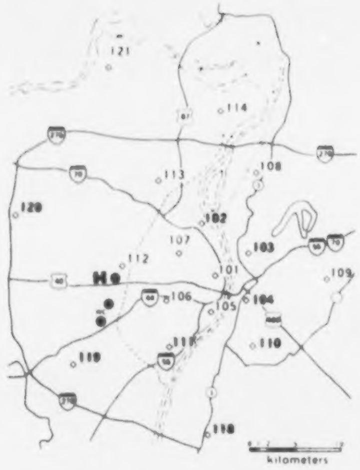
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Fig. 3A

Highway #40 Crossing

puff release time : 12:30 A.M.
puff crossing time: 12:55
tracer sample time: 12:57-1:04
calculated puff $\bar{c}$: 841 ppt
maximum measured c: 2787 ppt

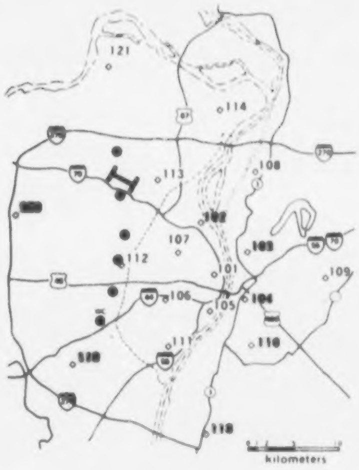
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Fig. 3B

Highway #70 Crossing

puff release time: 12:00 A.M.
puff crossing time: 1:00
tracer sample time: 12:51-1:02
calculated puff $\bar{c}$: 220 ppt
maximum measured c: 243 ppt

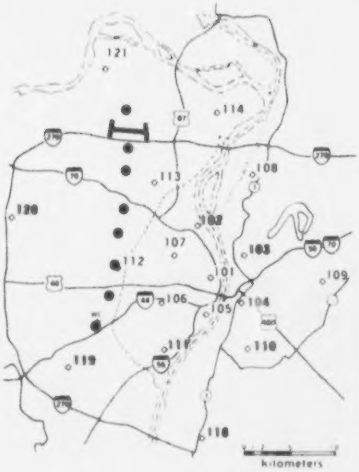
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Fig. 3C

Highway #270 Crossing

puff release time: 11:45 P.M.
puff crossing time: 1:15 A.M.
tracer sample time: 1:00-1:13
calculated puff $\bar{c}$: 122 ppt
maximum measured c: 183 ppt

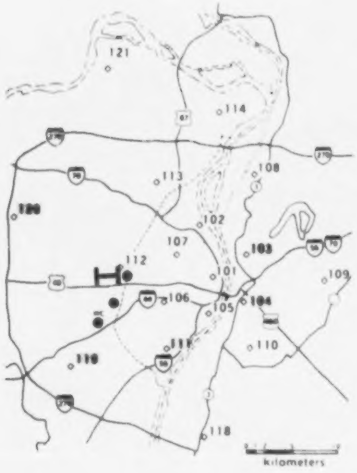
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Fig. 3D

Highway #40 Crossing

puff release time: 1:45 A.M.
puff crossing time: 2:10
tracer sample time: 2:20-2:26
calculated puff $\bar{c}$: 841 ppt
maximum measured c: 1961 ppt

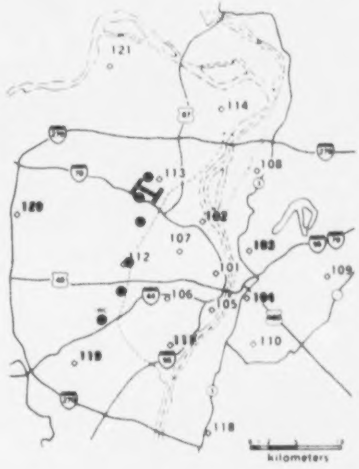
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Fig. 3E

Highway #70 Crossing

puff release time: 1:00 A.M.
puff crossing time: 1:50
tracer sample time: 2:01-2:12
calculated puff $\bar{c}$: 286 ppt
maximum measured c: 611 ppt

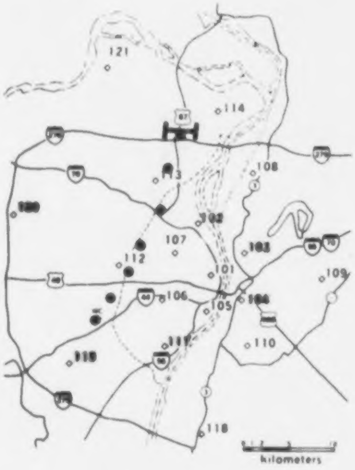
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Fig. 3F

Highway #270 Crossing

puff release time: 12:30 A.M.
puff crossing time: 2:00
tracer sample time: 2:08-2:20
calculated puff $\bar{c}$: 125 ppt
maximum measured c: 228 ppt

Puff Locations (dots) after 15-minute Intervals and Highway Traverses of SF_6 Plumes (Parallel bars)
August 12-13, 1975
St. Louis, Missouri

Note: ppt = parts per trillion

The puff released at 12:30 A.M. was transported across highway #270 near the intersection of highway #67, as shown in Fig. 3F. This was in agreement with the tracer study data. The puff was more than 20 km from the source point at this time. The calculated concentration was 125 ppt or 55% of the maximum concentration measured.

Four of the six puff trajectories presented here indicate that the model was spatially accurate in transporting the puffs across three highways in St. Louis. However, the temporal accuracy cannot be determined from the data used here, since the SF_6 tracer was emitted continuously. It should be noted, however, that both the tracer study and the transport model indicated that at approximately 2:00 A.M., the contaminant traversed a segment of highway #270 4-5 km to the east of the segment where the contaminant traversed the highway at approximately 1:15 A.M. (see Figs. 3C and 3F).

The remaining trajectories were approximately 1 km from the section of the highways where the tracer plume was detected by the instrumented automobile traverses. In these two cases, the puffs were transported across the grid in an area where data were missing from key RAMS sites #111 and #119. No data were available in the southwest corner of the grid, so the assumption was made that the 15-minute averaged wind velocity at RAPS sites #106 was representative of the averaged wind velocity at site #119. Therefore, the objective analyses of the wind was biased towards the wind velocity at site #106. This could have been the cause of the slight eastward displacement errors illustrated in Figs. 3A and 3D.

The concentrations calculated by the simple diffusion equation at the surface directly beneath the puffs were either comparable with or 2-3 times smaller than the maximum concentrations observed from the tracer study. The value of the diffusion coefficient in the diffusion equation was not calculated in this model. It was assigned a value thought to represent the atmospheric conditions at the time of the tracer study. Moreover, the amount of contaminant in the puff at its time of generation was arbitrarily defined by the amount of contaminant released during a one-minute time period. This diffusion calculation was a simple one and was used only to demonstrate an application of the transport model.

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THE CHANGE IN OZONE LEVELS CAUSED BY PRECURSOR POLLUTANTS:

AN EMPIRICAL ANALYSIS*

Leo Breiman
Technology Service Corporation
Santa Monica, CA. 90403

William S. Meisel
Technology Service Corporation
Santa Monica, CA. 90403

Abstract

An empirical analysis of ambient air data is used to relate the one-and two-hour change in oxidant levels in the urban environment to the preceding level of precursor pollutants and to meteorological variables. The intent was to demonstrate the feasibility of developing a set of empirical difference equations for the production of oxidant over time. The main variables determining one-and two-hour oxidant changes were extracted using nonparametric regression techniques. A model for two-hour oxidant changes was developed using nonlinear regression techniques. The implications of the model are discussed.

Introduction

Typical objectives of a modeling effort are (1) qualitative understanding and (2) quantitative impacts. In air quality modeling, these objectives are aimed at the ultimate objectives of determining the effects of alternative control policies and understanding which policies will be most productive. Ozone air quality modeling efforts have been largely concentrated at extremes of the spectrum of approaches to modeling: (1) simple statistical models with limited application, or (2) complex models based on the underlying physics and chemistry of the process. The former class of models provides easy-to-use, but rough, guidelines, the latter class of model is capable of detailed temporal and spatial impact analysis, but costly and difficult to use.

This paper illustrates the feasibility of an intermediate class of model which is relatively inexpensive and easy-to-use, but which is capable of providing reasonably detailed temporal and spatial estimates of oxidant concentration. Further, the form of the model makes it possible to understand (with careful inspection) the qualitative implications of the model as a guide to the design of control strategies.

We hasten to emphasize, however, that a full model in this class is not a result of this paper; rather, we present an analysis which we believe indicates the feasibility of the development of such a model. In particular, we develop an empirical difference equation for the production of oxidant from chemical precursors, as effected by meteorological variables. A full model would involve difference equations for the precursor pollutants as well. Further, data easily available did not include all meteorological variables of possible interest or emission data. (Since ozone is a secondary pollutant, emissions of primary pollutants over a brief interval, e.g., one hour, will not effect the change in ozone levels over that interval to the degree they effect the change in primary pollutant levels. Since we did not derive difference equations for the primary pollutants in this study, not including emissions did not prove serious.) The context in which the reader should then interpret the results is as the degree to which the change in ozone can be explained despite these limitations. Whatever degree of explanation of the variance in one- or two-hour changes in ozone we can achieve within these limitations can be improved when more of the omitted factors are taken into account. This analysis will thus provide a pessimistic estimate of the degree of success that can be expected in a full-scale implementation of the approach. This paper summarizes work reported more fully elsewhere [1].

Form of Model

We consider a "parcel" of air, and define $O_3(t)$ as the oxidant concentration averaged over the hour preceeding time t. We further define $\Delta O_3(t)$ as the change in the hourly average oxidant concentration (in pphm) in the time interval Δt following t; explicitly,

$$\Delta O_3(t) = O_3(t + \Delta t) - O_3(t) . \qquad (1)$$

(We will consider Δt = 1 hour and Δt = 2 hours.) We seek an equation predicting the change in hourly average concentration after time t from measurements of pollutants and meteorology available at time t. Pollutant measurements other than ozone we will consider as possible precursors include the following, all of them in terms of concentration averaged over the hour preceding time t:

$NO(t)$ = NO concentration (pphm)
$NO_2(t)$ = NO_2 concentration (pphm)
$HC(t)$ = Non-methane hydrocarbon concentration (ppm)
$CH_4(t)$ = Methane (ppm).

Meteorological variables considered explicitly include the following, again averaged over the hour preceding time t:

$SR(t)$ = solar radiation (gm-cal/cm^2/hrs)
$T(t)$ = temperature (°F).

Mixing height was not used in the present study.

We thus seek a relationship of the form

$$\Delta O_3(t) = F[O_3(t), NO(t), NO_2(t), HC(t), CH_4(t), SR(t), T(t)] \qquad (2)$$

which accurately reflects observed data. Referring to (1), equation (2) can be alternatively written as

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*This work was supported in part by Contract No. 68-02-1704 with the Environmental Protection Agency.

$$O_3(t + \Delta t) = O_3(t) + F\,[O_3(t),\ NO(t),\ NO_2(t),\ HC(t),\ CH_4(t),\ SR(t),\ T(t)].$$

This form indicates explicitly how such a relationship, if derived, can be used to compute a sequence of hourly or bi-hourly oxidant concentrations. (Similar equations would be derived for the primary pollutants to provide a complete model.)

We must incorporate transport effects. We have adopted a rather simple model. The model estimates the trajectory of a "parcel" of air from ground-level measurements of the wind field. A parcel arriving at a given location at a given time (e.g., Pasadena at 1600 hours) is estimated, from the current wind direction, to have been at another location upwind one hour earlier. The distance traveled from that direction is given by the current wind speed. The trajectory is tracked backwards to give a sequence of hourly locations. The "actual" values of pollutant levels at these points at the given times are obtained by an interpolation procedure from measured data at fixed monitoring stations. The motivation for tracking parcels backwards rather than forwards is to allow choice of parcels which end up at monitoring stations; in part so that the last (and often highest) pollutant concentration need not be interpolated. The air parcel trajectory approach is obviously a simplification of the true physics of the system; this approach is similar to assumptions employed in some physically based air quality models [2]. In the present empirical modeling context, the trajectory approach is a statistical approximation rather than an assumption; that is, the inaccuracy of the approximation will be reflected in the overall error of the final empirical model.

The Data

Data collected by the Los Angeles Air Pollution Control District was employed. Air quality data from the seven monitoring stations indicated in Figure 1 was utilized.

We interpolated the wind field in a region of the Los Angeles basin so that we were able to track parcels of air as they moved through the basin. The pollutant readings at seven APCD stations were also interpolated so that we could keep hourly records of the pollutants discussed. We also had the hourly solar radiation readings at the Los Angeles Civic Center location of the APCD, and hourly temperature readings at three representative locations in the basin.

Our study was carried out using data from the five summer months, June through October 1973. About 7000 trajectories were formed and placed in the primary data base.

From the bank of 7000 trajectories, we extracted a sample of about 1900 data vectors of the form

$$(\Delta O_3,\ O_3,\ NO,\ NO_2,\ HC,\ CH_4,\ SR,\ T)\ ,$$

where ΔO_3 was a one-hour change and about 1800 vectors where ΔO_3 was a two-hour change.

The Analysis

Since time is only implicit in (2), we search for a fixed relationship

$$\Delta O_3 = F(O_3,\ NO,\ NO_2,\ HC,\ CH_4,\ SR,\ T)\ . \qquad (4)$$

Equally important, we want to determine which of the variables were most significantly related to the change in ozone. Therefore, we really had two objectives in this study:

(1) To find those subgroups of the variables most significantly related to the ozone change.

(2) To find the form of the function F providing the best fit to the data.

Variable Selection

For the variable selection and exploratory phase, we used INVAR, a general nonparametric method for estimating efficiently how much of the variability in the dependent variable can be explained by a subgroup of the independent variables [3]. This technique estimates the limiting value of percent of variance explained (PVE) by a "smooth" nonlinear model.* We first tested all independent variables as individual predictors, then pairs of variables, and then added variables to find the best three, etc. Some results for single variables are tabulated in Table 1. The most significant individual variables (in approximate order of importance) are SR, NO_2, T, and O_3.

Exploring pairs of variables, we found the results shown in Table 2. Other pairs were run that resulted in lower percent of variance explained than those in the table.

Triplets of variables were then explored with one really significant improvement showing. Some results are shown in Table 3.

The final significant increase occurred when we added temperature to O_3, NO_2, SR. But, somewhat strangely, the increase was significant only for the data base of one hour ΔO_3. Here we obtained

Variables	One-Hour PVE
O_3, NO_2, SR, T	65.9

In all of the INVAR runs using HC and CH_4, neither of them significantly increased the PVE. For instance, when HC and CH_4 were individually added to the variables NO_2, NO, O_3, and SR, the maximum increase in PVE was 2.1%.

These results are encouraging; the three variables O_3, NO_2, SR predict about 71% of the variance in two-hour ozone changes, that is, with a correlation between predicted and actual values of 0.84 over 1800 samples.

Specific Functional Relationship

The exploratory analysis provided nonparametric estimates of the degree of predictability of two-hour ΔO_3 as a function of O_3, NO_2, SR. In this section,

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*Percent of variance explained equals

$$100 \times \left[1 - \frac{\text{variance of error in prediction}}{\text{variance of dependent variable}}\right]$$

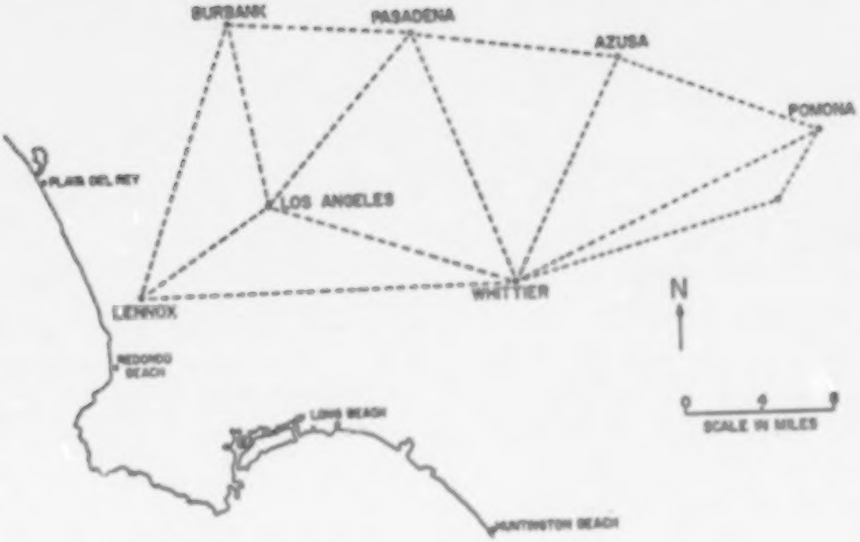

Figure 1. The Study Region.

Table 1. Percent of Variance Explained (Single Variables)

Variable	One-hour ΔO_3	Two-hour ΔO_3
O_3	15.8	24.1
NO	13.4	12.9
NO_2	25.7	41.7
HC	19.2	15.6
CH_4	16.6	19.3
SR	30.3	36.7
T	17.1	35.8

Table 2. Percent of Variance Explained (Pairs of Variables)

Variable	One-hour ΔO_3	Two-hour ΔO_3
NO_2, O_3	40.8	55.0
NO_2, SR	42.3	49.6
NO_2, T	38.7	52.9
NO_2, NO	34.8	50.1
O_3, SR	53.0	58.8
SR, T	43.6	52.1
O_3, T	33.2	46.7

Table 3. Percent of Variance Explained (Triplets of Variables)

Variables	One-hour ΔO_3	Two-hour ΔO_3
O_3, NO_2, SR	60.2	71.1
NO_2, NO, SR	46.7	53.8
O_3, NO_2, T	46.7	64.9

we discuss the derivation of a specific simple functional form to make explicit this relationship.

To get a continuous functional form for the relationship of ΔO_3 to O_3, NO_2, and SR, we used continuous piecewise linear regression [4,5]. Since the function generated by this method is smoother and less general than that used in INVAR estimates, we did not achieve the level of PVE obtained by INVAR. The continuous piecewise linear function which minimizes the mean-square error in the fit to the 1800 sample points is given by*

$$\Delta O_3 = -\,5.125 \cdot \max\,(A,B,C) - 1.167 \cdot \max\,(D,E,F) + 10.48 \qquad (5)$$

where:

$$A = -\,0.2146 \cdot O_3 - .0701 \cdot NO_2 - .002268 \cdot SR + .9376$$
$$B = .02114 \cdot O_3 - .1013 \cdot NO_2 - .01075 \cdot SR + 2.275$$
$$C = .1638 \cdot O_3 - .09855 \cdot NO_2 - .005938 \cdot SR - .2263$$

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*The notation max (A,B,C) means the largest of the three values computed by equations A, B, and C.

$$D = .02709 \cdot O_3 - .3015 \cdot NO_2 + .001298 \cdot SR + 2.304$$

$$E = -.009565 \cdot O_3 + .0005252 \cdot NO_2 - .001079 \cdot SR + .2306$$

$$F = -.0144 \cdot O_3 + .2066 \cdot NO_2 - .003171 \cdot SR - 2.943$$

(The unusual form of the equation has no physical interpretation, but is simply a consequence of the particular methodology employed.) This equation explained 60.7% of the variance, a correlation between predicted and actual values of 0.78.

This equation can be used to calculate a sequence of oxidant concentrations in a parcel of air by using known values of the other pollutant concentrations (since difference equations for these pollutants have not been derived). Figures 3, 4, and 5 illustrate the result for three air parcel trajectories.

INTERPRETATION OF MODEL IMPLICATIONS

Let us attempt to interpret the functional form in (5). The final fited surface is fairly simple, consisting of a continuous patching together of eight hyperplane segments. A three-dimensional slice of this surface is graphed in Figure 2. Of the eight regions, there are three small regions that together contain only 1.0% of the total number of points. We will ignore these and restrict our analysis to the information contained in the functional fit to ΔO_3 in the five other regions.

As a quick preliminary summary, in Table 4 we give the means of all variables corresponding to the points in each region.

Table 4. Means of Variables by Region

Region	Percent of Points	ΔO_3	O_3	NO_2	SR
Overall	100	7.1	6.1	9.0	100
Region 1	46	3.7	3.6	4.9	73
Region 2	33	11.0	4.6	11.9	118
Region 3	8	1.2	20.4	7.3	139
Region 4	7	14.7	5.4	20.3	119
Region 5	5	8.7	16.7	12.8	149

In Table 5 the mean values are characterized by region.

Table 5. Mean Value Characteristics

Region	ΔO_3	O_3	NO_2	SR
1	very low	very low	very low	very low
2	high	low	above avg.	above avg.
3	very low	high	below avg.	high
4	high	below avg.	high	above avg.
5	above avg.	high	above avg.	high

This layout of mean values is itself interesting. Region 1, containing almost half of the sample points, is representative of low pollution levels, low O_3 production, and low solar radiation. Region 2, with 33% of the points, contains data with above average mean NO_2 and solar radiation levels, below average O_3 levels, and high positive changes in O_3. The other three regions, with a total of 20% of the sample points, represent more extreme conditions.

The linear equations in each region are given in Table 6; these are derived from equation (5).

Table 6. Linear Equations for ΔO_3 by Subregion

Region	Equations			
1	$-.14\ (O_3)$	$+.87\ (NO_2)$	$+.054\ (SR)$	-3.9
2	$-.097(O_3)$	$+.52\ (NO_2)$	$+.056\ (SR)$	-1.4
3	$-.87\ (O_3)$	$+.86\ (NO_2)$	$+.029\ (SR)$	$+9.0$
4	$-.092(O_3)$	$+.28\ (NO_2)$	$+.059\ (SR)$	$+2.3$
5	$-.82\ (O_3)$	$+.26\ (NO_2)$	$+.034\ (SR)$	$+15.1$

Before discussing these results, since the size of the above coefficients depend on the scaling of the variables, we introduce normalized variables by dividing the original variables by their overall standard deviations, i.e., denoting normalized variables by primes:

$$O_3 = O_3/6.2,\ NO_2 = NO_2/5.2,\ SR = SR/52.8. \quad (6)$$

The equations are given in terms of the normalized variables, in Table 7.

Table 7. Normalized Equations for ΔO_3 (ΔO_3 not normalized)

Region	Equations			
1	$-0.9\ (O_3)$	$+4.5\ (NO_2)$	$+2.8\ (SR)$	-3.9
2	$-0.6\ (O_3)$	$+2.6\ (NO_2)$	$+2.9\ (SR)$	-1.4
3	$-5.4\ (O_3)$	$+4.4\ (NO_2)$	$+1.5\ (SR)$	$+9.0$
4	$-0.57(O_3)$	$+1.4\ (NO_2)$	$+3.1\ (SR)$	$+2.3$
5	$-5.1\ (O_3)$	$+1.4\ (NO_2)$	$+1.8\ (SR)$	$+15.1$

The major qualitative conclusions that can be inferred from these tables (see [1] for fuller discussion) are the following:

(1) At below average O_3 levels, the O_3 change is determined largely by the SR and NO_2 levels, with larger values of these latter two related to larger values of the O_3 change. The largest positive changes in O_3 occur in this regime.

(2) At above average O_3 levels, the O_3 has a strong negative association with O_3 change, and moderate to high levels of NO_2 and SR are associated with low to only moderately above-average changes in O_3.

Conclusion

We were able to derive surprisingly accurate equations predicting the short-term change in oxidant concentration (considering the limitations of the data and the difficulty of the problem). These results are encouraging in terms of the practicality of a full model involving emission variables and all the major reactive pollutants.

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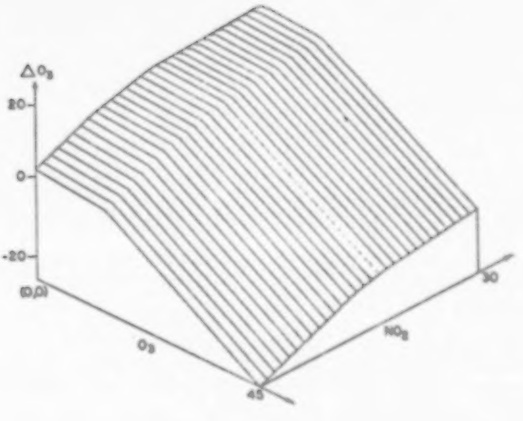
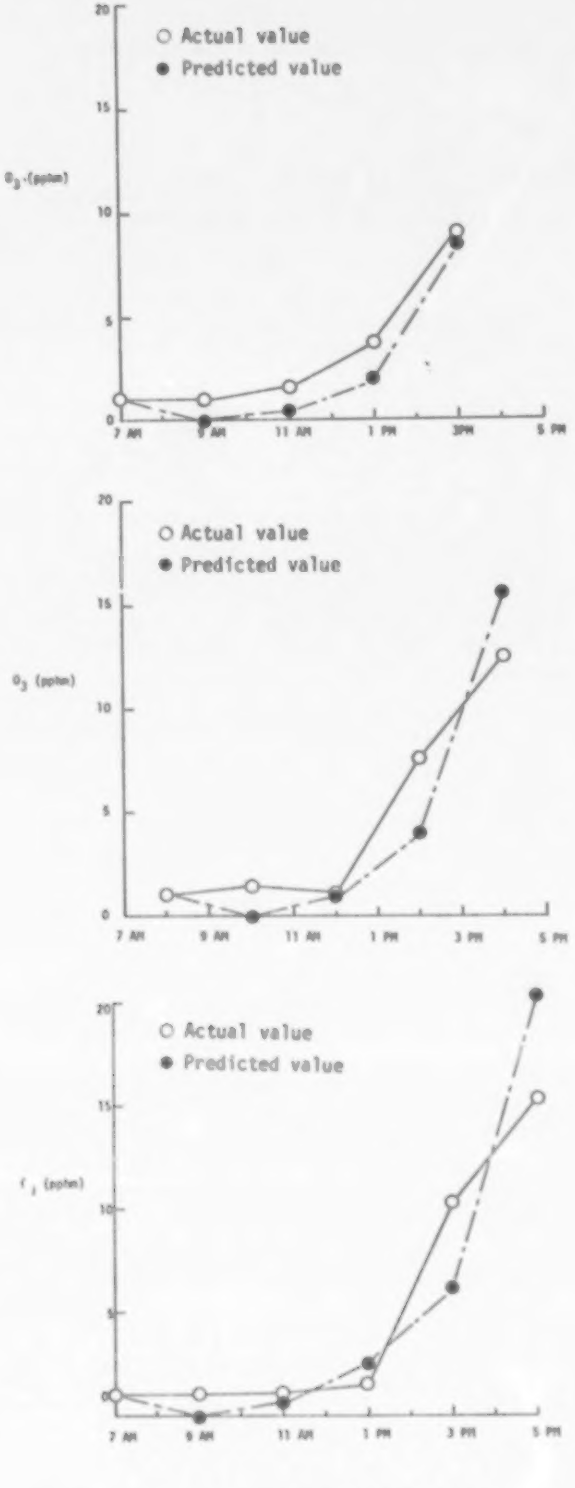


Figure 2. Graph of Regression Surface, with SR = 100.



Figures 3, 4, & 5. Wind Parcels Arriving at the Pomona Station at 3, 4, & 5 PM, respectively.

QUALITY ASSURANCE AND DATA VALIDATION FOR THE REGIONAL AIR MONITORING SYSTEM OF THE ST. LOUIS REGIONAL AIR POLLUTION STUDY

By

Robert B. Jurgens*
Environmental Sciences Research Laboratory
Research Triangle Park, North Carolina 27711

And

Raymond C. Rhodes
Environmental Monitoring and Support Laboratory
Research Triangle Park, North Carolina 27711

The success of model development and evaluation from a body of monitoring data depends heavily upon the quality of that data. The quality of the monitoring data in turn is dependent upon the various quality assurance (QA) activities which have been implemented for the entire system, commencing with the design, procurement, and installation of the system and ending with validation of monitoring data prior to archiving. Of the many sources of aerometric and emissions data that exist, the St. Louis Regional Air Pollution Study (RAPS) is the only known study specifically designed for model development and evaluation on an urban/rural scale.[1,2]

The prime objective of RAPS is to develop and evaluate mathematical models which will be useful in predicting air pollution concentrations from information of source emissions and meteorology. In addition to detailed emissions and meteorological data, an extensive base of high quality pollutant monitoring data is required to verify and to refine the models.

The Regional Air Monitoring System (RAMS) is the ground-based aerometric measurement system of RAPS and consists of 25 automated data acquisition sites situated in and about the St. Louis metropolitan area. Data from these 25 stations are transmitted over telephone lines to a central computer facility for processing and then sent to Research Triangle Park for archival. Details of RAMS have been described by Meyers and Reagan.[3] The complex air pollution, meteorological, and solar radiation measurements that are made at RAMS sites are shown in Table 1. Also shown are the recording intervals and the number of recording stations for each instrument.

Two main challenges exist for an effort of the magnitude of the St. Louis study:

1. To efficiently and effectively handle the large quantity of monitoring data; and

2. To obtain high quality monitoring data.

In general, data validity results from: (1) A quality assurance system aimed at acquiring acceptable data, and (2) A screening process to detect spurious values which exist in spite of the quality control process.

Table 1. RAMS NETWORK MEASUREMENTS

		MEASUREMENT INTERVAL (min)	NUMBER STATIONS
AIR QUALITY:	SULFUR DIOXIDE	5	13
	TOTAL SULFUR	1	12
		5	12
	HYDROGEN SULFIDE	5	13
	OZONE	1	25
	NITRIC OXIDE	1	25
	OXIDES OF NITROGEN	1	25
	NITROGEN DIOXIDE	1	25
	CARBON MONOXIDE	5	25
	METHANE	5	25
	TOTAL HYDROCARBONS	5	25
METEOROLOGICAL:	WIND SPEED	1	25
	WIND DIRECTION	1	25
	TEMPERATURE	1	25
	TEMPERATURE GRADIENT	1	7
	PRESSURE	1	7
	DEW POINT	1	25
	AEROSOL SCATTER	1	25
SOLAR RADIATION:	PYRANOMETER	1	6
	PYRHELIOMETER	1	4
	PYRGEOMETER	1	4

QUALITY ASSURANCE SYSTEM

The following list includes the elements of a total quality assurance system for aerometric monitoring:

- Quality policy
- *Quality objectives
- *Quality organization and responsibility
- QA manual
- *QA plans
- Training
- *Procurement control
    - Ordering
    - Receiving
    - Feedback and corrective action
- *Calibration
    - Standards
    - Procedures
- Internal QC checks
- Operations
    - Sampling
    - Sample handling
    - Analysis
- Data
    - Transmission
    - Computation
    - Recording
    - * Validation
- *Preventive maintenance
- *Reliability records and analysis
- *Document control
- *Configuration control
- *Audits
    - On-site system
    - Performance
- Corrective action
- Statistical analysis
- Quality reporting
- Quality investigation
- Interlab testing
- Quality costs

Detailed definition and discussion of the elements of quality assurance for air pollution measurement systems have recently been published.[4]

The elements of particular concern to RAMS[5] fall into three general categories:

1. Procurement and management, those activities which need to be established or accomplished early in the program;

2. Operation and maintenance, those activities which need to be performed routinely to assure continued operation of the system; and

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*On assignment from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce.

*These particular elements, of major concern to data screening, are discussed herein.

3. Specific data quality control activities, those activities which involve the calibration and data output from the meteorological and pollutant measurement instruments and are explicitly involved in acquiring quality data.

Procurement and Management

Data Quality Objectives. A requirement of the initial contract stated that 90% valid data were to be achieved. Valid data for pollutant measurements were defined as the data obtained during periods when the daily zero and span drifts were less than 2 per cent, with an allowance for the time required to perform daily zero/span checks and periodic multi-point calibrations.

Procurement. In planning to achieve the objectives very stringent requirements were placed on the suppliers of the various instruments of the system and extensive performance tests (with numerous rejections) were conducted prior to final acceptance.

First Article Configuration Inspection (FACI). The first remote station was installed and performance tested by the contractor under EPA review. Various indicated corrections were made before proceeding with the installation of the entire network.

System Acceptance Test (SAT). After installation of the entire network, a one-month system performance demonstration was required to assure satisfactory operation with respect to obtaining data of adequate quantity and quality. The SAT was completed in December 1974.

Incentive Contract. The current contract has introduced award fee performance incentives for management, schedule, and for quality. The quality portion of the award fee provides a continual motivation for obtaining and improving data quality.

Quality Assurance Plans. An extensive QA plan has been developed by the contractor. A point of emphasis is that the QA plan (and its implementation) is dynamic --continually being revised and improved based upon experience with the system. The QA plan outlines in detail the activities of the various QA elements previously mentioned.

Organization. To implement the QA plan, one full-time employee is assigned to overall QA responsibilities reporting directly to the Program Manager. In addition, two persons are assigned for QA on a half-time basis, one for the remote monitoring stations, and the other for the central computer facility.

Operation and Maintenance

Document Control. Detailed operation and maintenance manuals have been prepared for the remote stations and for the central computer facility. These manuals are issued in a loose-leaf revisable and document-control format so that needed additions and/or revisions can be made. Also, a complete history of changes are kept so that traceability to the procedures in effect for any past period of time can be made. A document control system also exists for the computer programs.

Preventive Maintenance. Record-keeping and appropriate analysis of the equipment failure records by instrument type and mode of failure have enabled more efficient and effective scheduling of maintenance and optimum spare parts inventory with resultant improvement in instrument performance. RAMS station preventive maintenance is completed twice each week. Normally, the remote stations are unattended except for the weekly checks, for other scheduled maintenance, or for special corrective maintenance.

Central Computer Monitors. Central computer personnel, using a CRT display, periodically monitor the output from all stations to detect problems as soon as possible. To maximize the satisfactory operation of the network equipment, the assigned QA personnel review the following activities associated with preventive maintenance:

1. remote station logbook entries,

2. remote station corrective maintenance reports,

3. laboratory corrective maintenance reports, and

4. central computer operator log.

Additionally, the QA individuals are in frequent verbal communication with field and laboratory supervisors to discuss quality aspects of the operations.

Reliability Records and Analysis

Telecommunications Status Summaries. Each day, a summary of telecommunications operations is prepared to determine which stations and/or telephone lines are experiencing significant problems that might require corrective action.

Daily Analog/Status Check Summaries. Each day, the central computer prepares a summary of analog/status checks by station so that major problems can be corrected as soon as possible by available field technicians. These analog/status checks are explained in the section on data validation.

Configuration Control. Histories are kept of the station assignment of specific instruments, by serial number, so that possible future problems with specific instruments can be traced back to the stations. A logbook for each instrument is maintained for recording in a systematic manner the nature and date of any changes or modifications to the hardware design of the instruments.

Specific Data Quality Control Activities

Calibration

Calibration References for Gaseous Pollutants. NBS standard reference materials are used for calibration standards if available. Otherwise, commercial gases are procured and certified at NBS for use as standards.

Multipoint Calibrations. As a check on the linearity of instrument response, an on-site, 5-point calibration is scheduled at each station at 8-week intervals. Originally, acceptability was determined by visual evaluation of the calibration data plots; more recently, quantitative criteria are being established for linearity.

Measurement Audits. Independent measurement audits for pollutant instruments are performed by the contractor using a portable calibration unit and independent calibration sources at each station once each calendar quarter. Similar audits are performed on the same frequency for temperature, radiation, and mass flowmeters; and independent checks are made on relative humidity, windspeed, and wind direction instruments. In addition to the internal audits performed by the contractor on his own operation, a number of external audits have been performed by EPA and other contractors[5] to check the entire measurement system.

On-Site System Audit. A thorough, on-site quality system audit of RAMS was performed for EPA by an independent contractor.[6] The results of this audit pointed out several areas of weakness for which corrective actions have been implemented.

Data Validation. As a part of the overall QA system, a number of data validation steps are implemented. Several data validation criteria and actions are built into the computer data acquisition system:

Status Checks. About 35 electrical checks are made to sense the condition of certain critical portions of the monitoring system and record an on-off status. For example, checks are made on power on/off, valve open/shut, instrument flame-out, air flow. When these checks are unacceptable, the corresponding monitoring data are automatically invalidated.

Analog Checks. Several conditions including reference voltage, permeation tube bath temperature, and calibration dilution gas flow are sensed and recorded as analog values. Acceptable limits for these checks have been determined, and, if exceeded, the corresponding affected monitoring are invalidated.

Zero/Span Checks. Each day, between 8-12 pm, each of the gaseous pollutant instruments in each station are zeroed and spanned by automatic, sequenced commands from the central computer. The results of the zero/span checks provide the basis for a two-point calibration equation, which is automatically computed by the central computer and is used for converting voltage outputs to pollutant concentrations for the following calendar day's data. In addition, the instrument drift at zero and span conditions between successive daily checks are computed by the central computer and used as a basis for validating the previous day's monitoring data. Originally, zero and span drifts were considered as acceptable if less than 2 per cent, but the span drift criterion has recently been increased to 5 per cent, a more realistic level. If the criteria are not met, the minute data for the previous day are flagged. Hourly averages are computed during routine data processing only with data which have not been flagged as invalid.

DATA SCREENING IN RAMS

The tests which are used to screen RAMS data are summarized in Table 2. Specific tests and associated data base flags are listed. The types of screens that have been employed or tested will be detailed, the mechanisms for flagging will be reviewed, and then the implementation of screening within RAMS will be discussed.

Table 2. SCREENING CATEGORIES AND ASSOCIATED FLAGS FOR RAMS DATA

Category	Flag
I. Modus Operandi	
No instrument	10^{17}
Missing measurement	10^{17}
Status	Value + 10^{-25}
Calibration	10^{35}
II. Continuity and Relational	
A. Intrastation	
Gaseous analyzer drift	- Value
Gross limits	10^{16}
Aggregate frequency distributions	Being implemented
Relationships	Value + 10^{32}
Temporal continuity	
Constant output	Value + 10^{23}
Successive difference	Being implemented
B. Interstation	
Meteorological network uniformity	Value + 10^{14}
Statistical outliers	
Dixon Ratio	Value + 10^{-20}
III. A Posteriori	
Review of station log	Invalidate 10^{18}
Unusual events or conditions	Validate - Remove Flag
Visual inspection of data	

For descriptive purposes, the tests are divided into three categories. The first category, "Modus Operandi," contains checks which document the network instrument configuration and operating mode of the recording system. Included are checks for station instrumentation, missing data, system analog and status sense bits, and instrument calibration mode. These checks, which have been described above, are part of the quality control program incorporated in the data acquisition system and central facility data processing, and are an important data management function used to document system performance.

The second category, "Continuity and Relational," contains temporal and spatial continuity checks and relational checks between parameters which are based on physical and instrumental considerations or on statistical patterns of the data. A natural subdivision can be made between intrastation checks, those checks which apply only to data from one station, and interstation checks, which test the measured parameters for uniformity across the RAMS network.

Intrastation checks include tests for gaseous analyzer drift, gross limits, aggregate frequency distributions, relationships, and temporal continuity. The drift calculations, which are part of the quality control program, have been discussed above.

Gross limits, which are used to screen impossible values, are based on the ranges of the recording instruments. These, together with the parametric relationships which check for internal consistency between values, are listed in Table 3. Setting limits for relationship tests requires a working knowledge of noise levels of the individual instruments. The relationships used are based on meteorology, atmospheric chemistry, or on the principle of chemical mass balance. For example, at a station for any given minute, TS cannot be less than $SO_2 + H_2S$ with allowances for noise limits of the instruments.

Table 3. GROSS LIMITS AND RELATIONAL CHECKS

PARAMETER	INSTRUMENTAL OR NATURAL LIMITS		INTERPARAMETER CONDITION
	LOWER	UPPER	
Ozone	0 ppm	5 ppm	$NO*O_3 \leq 0.04$
Nitric Oxide	0 ppm	5 ppm	$NO - NO_x \leq$ Noise (NO)
Oxides of Nitrogen	0 ppm	5 ppm	$NO - NO_x \leq$ Noise (NO_x)
Carbon Monoxide	0 ppm	50 ppm	
Methane	0 ppm	50 ppm	CH_4 - THC ≤ Noise (CH_4)
Total Hydrocarbons	0 ppm	50 ppm	CH_4 - THC ≤ Noise (THC)
Sulfur Dioxide	0 ppm	1 ppm	SO_2 - TS ≤ Noise (SO_2)
Total Sulfur	0 ppm	1 ppm	SO_2 - TS ≤ Noise (TS)
Hydrogen Sulfide	0 ppm	1 ppm	H_2S - TS ≤ Noise (H_2S)
Aerosol Scatter	$0.000001m^{-1}$	$0.00099m^{-1}$	
Wind Speed	0 m/s	22.2 m/s	
Wind Direction	0°	360°	
Temperature	-20°C	45°C	
Dew Point	-30°C	45°C	DP - 0.5 ≤ T
Temperature Gradient	- 5°C	5°C	
Barometric Pressure	950 mb	1050 mb	
Pyranometers	- 0.50	2.50 Langleys/min	
Pyrgeometers	0.30	0.75 Langleys/min	
Pyrheliometers	-0.50	2.50 Langleys/min	

A refinement of the gross limit checks can be made using angregate frequency distributions. With a knowledge of the underlying distribution, statistical limits can be found which have narrower bounds than the gross limits and which represent measurement levels that are rarely exceeded. A method for fitting a parametric probability model to the underlying distribution has been developed by Dr. Wayne Ott of EPA's Office of Research and Development.[7]. B.E. Suta and G.V. Lucha[8] have extended Dr. Ott's program to estimate parameters, perform goodness-of-fit tests, and calculate quality control limits for the normal distribution, 2- and 3-parameter lognormal distribution, the gamma distribution, and the Weibull distribution. These programs have been implemented on the OSI computer in Washington and tested on water quality data from STORET. This technique is being studied for possible use in RAMS as a test for potential recording irregularities as well as a refinement of the gross limit check currently employed.

Under intrastation checks are specific tests which examine the temporal continuity of the data as output from each sensor. It is useful to consider, in general, the types of atypical or erratic responses that can occur from sensors and data acquisition systems. Figure 1 illustrates graphically examples of such behavior, all of which have occurred to some extent within RAMS. Physical causes for these reactions include sudden discrete changes in component operating characterisitcs, component failure, noise, telecommunication errors and outages, and errors in software associated with the data acquisition system or data processing. For example, it was recognized early in the RAMS program that a constant voltage output from a sensor indicated mechanical or electrical failures in the sensor instrumentation. One of the first screens that was implemented was to check for 10 minutes of constant output from each sensor. Barometric pressure is not among the parameters tested since it can remain constant (to the number of digits recorded) for periods much longer than 10 minutes. The test was modified for other parameters which reach a low constant background level during night-time hours.

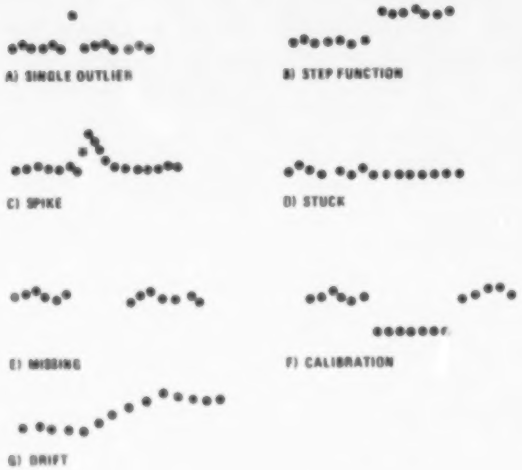

Figure 1. Irregular instrument response.

A technique which can detect any sudden jump in the response of an instrument, whether it is from an individual outlier, step function or spike, is the comparison of minute successive differences with predetermined control limits. These limits are determined for each parameter from the distribution of successive differences for that parameter. These differences will be approximately normally distributed with mean zero (and computed variance) when taken over a sufficiently long time series of measurements.

Exploratory application of successive differences, using 4 standard deviation limits which will flag 6 values in 100,000 if the differences are truly normally distributed, indicate that there are abnormal occurrences of "jumps" within certain parameters. Successive difference screening will be implemented after further testing to examine the sensitivity of successive difference distributions to varying computational time-periods and to station location.

The type of "jump" can easily be identified. A single outlier will have a large successive difference followed by another about the same magnitude but of opposite sign. A step function will not have a return, and a spike will have a succession of large successive differences of one sign followed by those of opposite sign.

The interstation or network uniformity screening tests that have been implemented in RAMS will now be described. Meteorological network tests are performed on hourly average data and are based on the principle that meteorological parameters should show limited differences between stations under certain definable conditions typically found in winds of at least moderate speeds (>4 m/sec). Each station value is compared with the network mean. The network mean is defined as the average value for a given parameter from all stations having reported valid data. (If more than 50% are missing, a network mean is not computed and the test is not made.) Values exceeding prescribed limits are flagged. The limits have been set on the advice of experienced meteorologists. The tested parameters and flagging limits are listed below.

Maximum allowable deviations from network mean under moderate winds (network mean $\geq$ 4 m/sec)

Wind speed	2 m/sec or MEAN/3 (whichever is larger)
Wind direction	30^{0}
Temperature	3^{0}C
Temperature difference	$.5^{0}$C
Dew point	3^{0}C
Adjusted pressure	5.0 millibars

In addition to network screening techniques which are based on knowledge of underlying physical processes, methods from statistical outlier theory[9,10] were also examined. Specifically, the Dixon ratio test[11] was implemented to determine extreme observations of a parameter across the RAMS network. The Dixon ratio test is based entirely on ratios of differences between observations from an assumed normal distribution and is easy to calculate. The Dixon criteria for testing a low suspect value from a sample size of n, $n \leq 25$, are shown in Figure 2. Though the entire sample is shown as ranked, only the extreme 2 or 3 values need to be ordered. Associated with each value of n are tabulated ratios for statistical significance at various probability levels. For example, if n=25, X_1 would be considered as an outlier at the 1% level of significance when $r_{22} \geq .489$. Since the underlying distribution may not be normal, the calculated probabilities may not be exact, but are used as indicators of heterogeneity of the network observations at a given time.

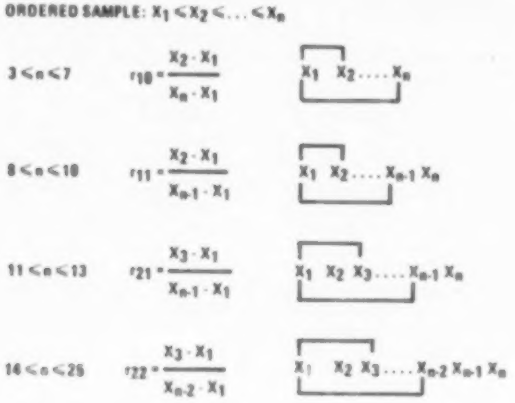
ORDERED SAMPLE: $X_1 \leq X_2 \leq \ldots \leq X_n$
$3 \leq n \leq 7$
$r_{10} = \frac{X_2 - X_1}{X_n - X_1}$
$X_1 \; X_2 \ldots X_n$
$8 \leq n \leq 10$
$r_{11} = \frac{X_2 - X_1}{X_{n-1} - X_1}$
$X_1 \; X_2 \ldots X_{n-1} \; X_n$
$11 \leq n \leq 13$
$r_{21} = \frac{X_3 - X_1}{X_{n-1} - X_1}$
$X_1 \; X_2 \; X_3 \ldots X_{n-1} \; X_n$
$14 \leq n \leq 25$
$r_{22} = \frac{X_3 - X_1}{X_{n-2} - X_1}$
$X_1 \; X_2 \; X_3 \ldots X_{n-2} \; X_{n-1} \; X_n$

Figure 2. Dixon ratio test for suspected low value.

The third screening category, a Posteriori, was established to provide a mechanism for overriding the automated flagging schemes which have been implemented in the instrumentation at the remote sites and in the data screening module. From a review of station logs and preventive maintenance records, a knowledge of unusual events, or through visual inspection of data, it may be determined that previously valid data should be flagged as questionable. Conversely, it may be determined that previously invalid data should be validated by removing existing flags. An example of when data would be invalidated is when an instrument, such as a wind direction indicator, becomes misaligned or uncalibrated because of some non-linear or unknown reason. Removal of flags or revalidation can occur, for example, when the recording instruments function properly, but the sense bit or analog status circuity is known to have malfunctioned.

Implementation of a posteriori changes of RAMS data requires special software, inserted in the data flow during data processing, screening and archiving, or during a special pass through the data after archival.

Data Flagging

Embedded in the data base structure must be a flagging mechanism which can distinguish the various data screens. In general, data which have been filtered by the various screens must be either removed from the data base or qualified by attaching a uniquely identifying flag.

Two details of the RAMS archival data base are important to understanding the implementation of the RAMS data flagging. First, all data are stored in integer floating point numbers in Univac internal binary representation. Floating point notation is a natural representation of numerical data and can readily accommodate a variety of flagging schemes. Second, each potential measurement has a reserved location in the data base. Thus, substitutions must be made for missing and removed data. For instance, RAMS data rejected by the gross limit checks are removed and replaced by a value of 10^{34}.

Data which have been screened and which are not obviously impossible may have limited application and should not be eliminated from the data base. If each screening test can be associated with a unique flag, then modelers and other users can establish their own criteria for accepting or rejecting the flagged data.

Three flagging mechanisms suggest themselves when the value of the measurement is to be retained: (1) exponent offset, (2) range offset, and (3) binary bit encoding. These techniques are listed for reference only. A full description and comparison of these techniques is being prepared.

Exponent offsetting which is used for RAMS data is accomplished by multiplying the value by a power of 10. Special considerations must be given to the dynamic range of the data and to values which are identically zero. The flags which are associated with each of the individual screens are listed in Table 2.

Implementing the Screening Module Into the Data Flow

We emphasize the importance of considering the sequence in which screening is integrated into the data flow by considering a generalized data flow diagram, or basic system design, which is applicable to any environmental measurement system. This flow diagram is illustrated in Figure 3.

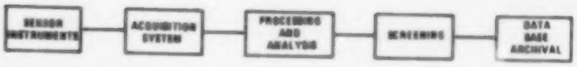

Figure 3. Generalized data flow for environmental measurement systems.

Data screening should take place as near to data acquisition as possible either in data processing which is traditionally concerned with laboratory analysis, conversion to engineering units, transcribing intermediate results, etc., or in a separate module, as illustrated, designed specifically for the screening process. Screening data soon after data acquisition permits system feedback in the form of corrective maintenance, changes to control processes, and even to changes in system design. This feedback is essential to minimize the amount of lost or marginally acceptable data.

The RAMS screening tests, which have been developed at Research Triangle Park (RTP), are now part of the data processing carried out at the RAPS central facility in St. Louis. Slow computation speeds of the St. Louis PDP 11/40 computer required restricting the intrastation screening tests to hourly average data. RAMS data is still passed through the RTP screening module before archiving.

SUMMARY

The experiences gained in RAMS and applicable to other monitoring systems are:

1. Data validity is a function of quality assurance and data screening.

2. A QA plan and data screening rules should be established initially and maintained throughout the program.

3. The QA plan and screening rules are dynamic, being improved as additional knowledge and experience is gained.

4. Applied during data acquisition or shortly thereafter, quality control and screening checks constitute an important feedback mechanism, indicating a requirement for corrective action.

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QUANTITATIVE RISK ASSESSMENT FOR COMMUNITY EXPOSURE TO VINYL CHLORIDE

Arnold M. Kuzmack
Office of Planning and Evaluation
U.S. Environmental Protection Agency
Washington, D.C. 20460

Robert E. McGaughy
Office of Health and Ecological Effects
U.S. Environmental Protection Agency
Washington, D.C. 20460

Summary

Vinyl chloride is a known human carcinogen; it has produced liver angiosarcoma, a very rare form of cancer, as well as other cancers and non-cancer effects in occupationally exposed populations. It is also known to be emitted into the atmosphere from plants which produce vinyl chloride monomer (VCM plants) and plants which polymerize the monomer to polyvinyl chloride (PVC plants). Although concentrations of vinyl chloride in the ambient air are much less than those which caused cancer in workers, it is generally considered prudent to assume that there is no threshold for chemical carcinogens, so that any exposure involves some risk. In conjunction with EPA consideration of rulemaking action to regulate emissions of vinyl chloride from VCM and PVC plants, the Administrator of EPA requested that an analysis be performed which would estimate quantitatively the risk resulting from VC emissions and assess the reliability of the estimates. This paper reports the results of that analysis. The details are presented in Appendices A through E, which are available from the authors on request.

Method of Analysis

The analysis involves three steps which are discussed below. They are an estimate of size of the exposed population, concentrations of vinyl chloride to which it is exposed, and number of liver angiosarcomas and other health effects which would result from this exposure. Of these, the last estimate is by far the most difficult to make. In addition, an investigation was made of the places of residence of all people known to have died of liver angiosarcoma in the last 10 years in an attempt to detect clustering around PVC and VC plants.

Although excess birth defects have been reported in communities near some plants, the current data is too fragmentary for conclusions to be drawn; thus, these effects have not been considered in this paper.

Size of Exposed Population

A study[1] by the American Public Health Association (APHA), performed under contract to EPA's Office of Toxic Substances, determined the number of people living within various distances, up to 5 miles, from each of 9 VCM plants and 33 PVC plants. The study was based primarily on census tract information. The validity of the methodology used was confirmed by a more detailed analysis of the population living around a few plants, performed by EPA's Office of Planning and Evaluation.

The total population living within 5 miles of all PVC and VCM plants is shown in the following table:

Distance (mi)	Population
0 - 1/2	47,000
1/2 - 1	203,000
1 - 3	1,491,000
3 - 5	2,838,000
TOTAL	4,579,000

Thus, a total of 4.6 million people live in the vicinity of these plants. The use of residence data involves some error, of course, since people spend part of their time away from their homes and are exposed to varying levels of vinyl chloride. There does not seem to be any practical way around this problem, short of a detailed study of travel patterns of 4 million people in over 40 separate communities.

Ambient Vinyl Chloride Concentrations

Annual average ambient concentrations of vinyl chloride were calculated by standard diffusion modeling techniques. Two independent studies were made, one by EPA's Office of Air Quality Planning and Standards (OAQPS) and one by Teknekron, Inc.[2] The agreement among the two studies was good, with differences generally less than 25%. It was decided to use the Teknekron results in the actual calculations since they included data on variations in meteorological conditions from location to location.

For an average uncontrolled PVC or VCM plant in an area with average meteorological conditions, the annual average concentration of vinyl chloride in each annulus around the plant is shown in the following table:

Distance (mi)	Vinyl Chloride Concentration (ppb)	
	PVC Plant	VCM Plant
0 - 1/2	323	113
1/2 - 1	57	20
1 - 3	15	5.2
3 - 5	5.7	2.0

It can be seen that concentrations around VCM plants are significantly smaller than around PVC plants. This fact combined with the much smaller population living near VCM plants implies that by far the greatest part of the public health risk is from emissions of PVC plants.

In calculating the average population exposure, it is necessary to consider, for each population affected, the type of plant (VCM or PVC), the size of plant, the multiplicity of plants nearby, and the meterological conditions at the plant site. Information from OAQPS and from the APHA study was used to determine areas where more than one plant was located, and OAQPS characterized the size of each plant as "average" or "large." The Teknekron study was used to categorize the meteorological and topographic conditions at each location.

The net result of these calculations is that the average exposure faced by a person chosen at random from the 4.6 million people living within 5 miles of plants is 17 ppb.

Unfortunately, it has not been possible to make a systematic comparison of the diffusion modeling results with data obtained from actual monitoring, although they appear generally consistent. It is therefore difficult to estimate the uncertainty of these estimates. Lacking anything better, we can take the difference between the two diffusion modeling efforts of up to 25% as an estimate of that uncertainty.

Health Effects Resulting From Exposure

What are the results of exposing 4.6 million people to an average of 17 ppb of vinyl chloride? The first major decision to face in answering this question is to arrive at some combination of two basic approaches. One approach is to rely largely on human data (which exists for vinyl chloride but not for many other chemicals of concern to EPA); the second is to make projections from animal experiments. Both involve difficulties. Use of human data eliminates the uncertainties that result because we do not know the differences in response between the test animals and humans. On the other hand, with the data on human (occupational) exposure, it is necessary to guess at exposure levels over the past 30 years and approximate the total number of workers involved and the number of cancers caused by past exposures for which symptoms may not appear until many years in the future. By using animal data we can avoid these problems, but only at the price of uncertainty in the relevance of animal experiments to human exposures. The approach taken in this analysis is to use animal data to predict the probability of human liver angiosarcoma, and then use the human data to the greatest extent possible to interpret those predictions.

A second major decision that must be made is how to project the results observed at high doses in animal experiments and in the occupational exposures to the much lower doses encountered in the environment. Two alternative assumptions are frequently made in the scientific literature. The first is a straight-line projection to zero dose, assuming no threshold (the "linear model"). This is also referred to as the "one hit" model, since it would follow logically from the assumption that each minute increment of exposure to a carcinogen has the same independent probability of causing a cancer, regardless of the dose level. This assumption is generally accepted as prudent in radiation carcinogenesis. For chemical carcinogenesis, the model is usually considered to provide an upper limit to the level of effects likely at extremely low doses, because the existence of detoxification mechanisms would render small doses less effective in causing cancer and would therefore result in a threshold, or at least fewer effects.

The second commonly used projection method is based on the assumption that the observed changes in response with dose are the result of variations of susceptibility in the population, which is assumed to be log-normally distributed with dose. For convenience, we refer to this as the "log-probit" model because it forms a straight line when the logarithm of the dose is plotted against the proportion of responses expressed in probability units (probits). The log-probit model is used in the Mantel-Bryan procedure.

In this analysis, both models are used. For technical reasons, the log-probit model is difficult to apply to this case. Therefore, the basic calculations were done using the linear model, but a sensitivity analysis was done to show how the results would change under the log-probit assumption. Thus, the log-probit model results are shown below as a range, not a definite number.

A third decision that must be made is how to predict human incidence rates from animal data. Again, there is little hard data to provide guidance. The assumption used here is that a lifetime exposure of humans to a given concentration of vinyl chloride would produce effects in the same proportion of individuals as a lifetime exposure of rats. Thus, the one-year exposure in the animal experiments would be equivalent to about 30 years of exposure for humans.

A fourth decision to make is how to use the available human data on liver angiosarcoma cases among highly-exposed workers to calculate the probability per year of exposure that cases will eventually develop in people. This calculation is needed for comparisons with the animal model. There are three aspects to this problem: 1) to find in the literature a realistic estimate for the fraction of highly-exposed workers who have contracted liver angiosarcoma at some time in their lives, 2) to account for the fact that the currently-observed rates underestimate the actual incidence because they do not include workers who have been exposed more recently than 15 to 20 years ago, and 3) to account for the fact that people can die from other causes before a latent case of liver angiosarcoma becomes manifest.

These issues were treated as follows: Of the four occupational epidemiology studies from which it is possible to estimate an incidence rate,[3-6] the two with the smallest number of subjects and the best separation of highly-exposed workers from the group of all workers[5,6] had the largest incidence of angiosarcoma. This incidence was assumed to be valid for all highly-exposed workers. The latency time distribution for liver angiosarcoma and the growth in the number of person-years of exposure since 1940 are two factors which affect the number of cases we have observed through 1974. These factors are analyzed in Appendix D. The result of the analysis is an estimate of the probability per year of exposure that a person will get angiosarcoma some time in his life. The remaining problem of multiple risks competing for mortality was not treated because of its complexity.

A fifth decision that must be made is how to quantatively describe the other effects of vinyl chloride exposure besides liver angiosarcoma. This problem was handled by estimating from the literature[3,7-9] ratios of the number of people with other cancers and the number of people with liver damage compared to the number with angiosarcoma. As an index of liver damage, the bromsulphalein (BSP) test is used because it, among all liver function tests that have been used, correlates best with vinyl chloride exposure and because an abnormal BSP test indicates that severe damage has occurred in the liver, either because the liver cells are not able to assimilate the intravenously injected BSP dye from the blood and excrete it into the bile passages, or that the bile passages are no longer structurally intact enough to carry the dye out of the liver.

Results of Analysis

The results of these five aspects of the problem are presented below in reverse order. The approximate ratio of severe liver damage cases to liver angiosarcoma cases is about 30, the result being consistent for two independent occupational studies. It was also found that about twice as many cases of cancer of all sites are caused by vinyl chloride as cases of liver angiosarcoma alone. The animal experiments have shown approximately the same ratio of all cancers to liver angiosarcoma, after background incidence is taken into account.

In calculating the probability per year of exposure that a highly-exposed worker will get angiosarcoma some time in his life, we found that the fraction of highly-exposed workers who have been currently diagnosed is 0.02. They have been exposed for an average of 17 years before diagnosis. The analysis, which was based on the available data on the time distribution of person-years of exposure and the distribution of latency times from first exposure to diagnosis, showed that only about 40% of the highly-exposed workers who are expected to get angiosarcoma some time in their lives have been diagnosed already. Since the data was incomplete, several assumptions had to be made in order to complete the analysis. Therefore, the probability that one of these people will get angiosarcoma some time in their lives is 0.02/(17 x 0.40) = 0.003 per year of exposure. In Appendix D, the calculation is explained in greater detail.

The 17-year average concentration to which these workers were exposed was estimated to be 350 ppm on the basis of one study. Only one company has reported measurements of vinyl chloride for the jobs in their plant. These measurements, started in 1950, show the highest exposure jobs ranged from 120 to 385 ppm before 1960, when the exposures were reduced because of suspected toxicological problems with vinyl chloride. In estimating the average, it was assumed that the other factories, most of which probably did not monitor the concentration of vinyl chloride, were less concerned about industrial hygiene and, therefore, took fewer precautions to keep the levels low.

In predicting the human angiosarcoma rate from the animal dose-response data, it was projected, from the linear model, that exposure to vinyl chloride would cause 0.071 cases of liver angiosarcoma and 0.15 cases of all types of cancer per million people per year per ppb of continuous exposure. Details of these calculations are given in Appendix B. Converting to a 7-hour per day, 5-day per week work schedule of exposure to 350 ppm, the model predicts an angiosarcoma incidence rate of 0.0052 per person-year exposure. It is shown in Appendix D that this rate is numerically indistinguishable from the rate of 0.003 calculated from the human data, considering the known quantifiable errors of estimating the parameters of the animal and human data. It can be concluded that the slope of the linear animal dose-response relationship for angiosarcomas is consistent with the human data.

The extrapolation of the animal dose-response relationship to a concentration of 17 ppb (the average concentration around the uncontrolled plants) yields the following predicted number of cases in the 4.6 million people living within 5 miles of the plants. For details, see Appendix B.

Type of Effect	Cases Per Year of Exposure	
	Linear Model	Log-Probit Model
All cancer	11	0.1 - 1.0
Liver angiosarcoma	5.5	0.05 - 0.5

This is the expected number of cases projected to be caused per year at current levels of emissions; the people exposed now will not be diagnosed for another 15-20 years. Similarly, any cases observed now would have been caused by exposure 15-20 years ago (if in fact caused by vinyl chloride) when production was about 10% of current levels.

In order to arrive at a final estimate of the number of people adversely affected by vinyl chloride emissions, the important results of this analysis to consider are as follows: 1) the number of cancers at all sites caused by vinyl chloride is twice the number of liver angiosarcomas; 2) the number of people with severe liver damage is 30 times the number of liver angiosarcomas; 3) the animal model predicts that the number of liver angiosarcomas in the population around plants is 5.5 cases per year of exposure; 4) the number of cases calculated from the human data is 60% of the number predicted from the animal model; 5) the use of a log-probit model for extrapolation to low doses gives predictions of 0.1 to 0.01 times the number predicted by the linear model; 6) the error in the estimate of 5.5 cases per year ranges from +55% to -10%. This error includes statistical uncertainty in estimating the dose-response, uncertainty in ambient concentration estimates, and errors resulting from not considering exposures beyond 5 miles or decomposition of vinyl chloride in the atmosphere. It is not symmetrical because it includes possible effects beyond 5 miles from the plants, which were not explicitly considered in the analysis. It does not account for our uncertainty about the appropriateness of using a linear model extrapolated to zero dose or of extrapolation from animal data; 7) the quantifiable error in the rate calculated from the human data is about ± 67%. This includes uncertainties in the 17-year average dose received by the workers, uncertainty in the number of hours per day of actual high exposure, and uncertainty in the fraction of highly-exposed workers who have been diagnosed with liver angiosarcoma. Other errors cannot be quantified, and are discussed in Appendix D.

Conclusions

When all these uncertainties are considered, our judgment is that the number of liver angiosarcoma cases produced per year of exposure in people residing near vinyl chloride plants is somewhere between less than 1 and 10 cases. The cases produced by this year's exposure will not be diagnosed until 15 to 20 years from now. If the EPA regulations are implemented, the number of cases is expected to be reduced in proportion to the reduction in the ambient annual average concentration, which is expected to be 5% of the uncontrolled level.

The vinyl chloride exposure around plants is also producing somewhere between less than 1 and 10 cases of primary cancer at other sites, mainly lung, brain, and bone. Assuming no threshold for liver damage, somewhere between less than 1 and 300 cases of serious liver damage would be predicted. The number of liver damage cases is likely to be less than this because a liver damage threshold at low dose probably exists.

In order to find out whether people living near VC-PVC plants have, as of 1974, had higher rates of liver angiosarcoma diagnosis than the overall U.S. population, a search of the residence records of all known liver angiosarcoma cases in the last 10 years was performed using data collected by the Center for Disease Control. Out of 176 cases where residence at time of death was known, 3 people lived within 5 miles of a plant. Unfortunately, the diagnosis of these cases has not yet been confirmed by the National Cancer Institute. In addition one infant whose parents lived within 1 mile of a plant died of a relatively common liver tumor. It was shown in Appendix E that this rate of occurrence is not higher than the national average. However, the survey is too incomplete to draw any conclusions at the current time.

Considering the results of the foregoing analysis, one would only now expect to be seeing some evidence of vinyl chloride exposure. If the highest rate in our range were actually occurring, 10 cases of liver angiosarcoma per year of exposure would be developing; 15-20 years ago when the vinyl chloride production was about 10% of current levels, one case would be expected per year of exposure (with constant population). This is to be compared to a background rate of 0.6 cases per year expected in the population around the plant.

The survey of liver angiosarcoma cases would probably detect the existence of 10 cases over the 10-year period. Since this was not observed we can conclude that the real incidence is not significantly greater than the predicted upper limit of 10 cases initiated per year of exposure unless migration of people in and out of the regions around plants has been excessive. If the lower rates in the range of the above analysis were to be true, increased incidence of angiosarcoma would not be observable.

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NEW MODELS FOR OPTIMAL SEWER SYSTEM DESIGN

Ben Chie Yen
Harry C. Wenzel, Jr.
Larry W. Mays
Wilson H. Tang
Department of Civil Engineering
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801

SUMMARY

Three new models have been developed for the least-cost design of storm sewers. All three models consider the sewers as a system. The basic model designs the crown elevations, slopes, and diameters of the sewers. The sewer system layout is predetermined. Routing is accomplished by lagging the hydrographs by a travel time. Optimization is achieved through a discrete differential dynamic programming technique to produce the least-cost design of the system based on specified cost functions for installation of the sewers and manholes. The second model is an expansion of the basic model incorporating risk-based damage costs in the design procedure, and the risks for each sewer associated with the least-cost design are also given as part of the design results. The third model is similar to the basic model except that the least-cost sewer layout is also a part of the design result instead of being predetermined.

INTRODUCTION

Urban storm sewer simulation models can be classified into two basic categories. The majority are flow simulation models for existing systems. They are useful for urban storm runoff management, operation and pollution control purposes by providing information useful for flow regulation. Many of these models have been mislabeled as "design" models whereas in fact they produce nothing more than runoff hydrographs that may be used for design. Evaluations of the important flow simulation models have been reported by Chow and Yen[6], Brandstetter[3], James F. MacLaren, Ltd.[5], and others.

The second category are design models for determination of the size, and perhaps also slopes and layout of the sewers. There are only a few design models in existence. A comparative study of hydraulic design models was reported by Yen and Sevuk[10]. These models determine the sewer sizes with predetermined sewer slopes and layout. Recently a number of optimization models for the least-cost design of sewer systems have been proposed and a review has been reported by the authors[12]. Most of these models offer a limited degree of optimization in determining the sizes and slopes of sewers using linear programming or dynamic programming.

In this paper three new sewer design models are reported. An optimization procedure is incorporated into each of the models to determine the least-cost design for the entire sewer system. The first model employs a simple hydrograph shift routing scheme and determines the crown elevations, slopes, and diameters of the sewers. The second model is based on the first, however the uncertainties and risks are considered in the design procedure. The third model is similar to the first in its scope and extent except that it also determines the layout of the sewer system. In the following the constraints, assumptions and basic optimization techniques adopted in all the three models are first discussed. The three design models developed and listed in Table 1 are then described briefly. Finally an example is presented to illustrate the advantages of the new design models over the traditional design methods.

CONSTRAINTS AND ASSUMPTIONS

The following constaints commonly used in sewer designs[2] are adopted in this study:

(a) Free-surface flow exists for the design discharges or hydrographs, i.e., the sewer system is "gravity flow" so that pumping stations and pressurized sewers are not considered.
(b) The sewers are commercially available circular sizes no smaller than 8 in. in diameter. The pipe sizes in inches are 8, 10, 12, from 15 to 30 with a 3 in. increment and from 36 to 120 with an increment of 6 in.
(c) The design diameter is the smallest commercially available pipe that has flow capacity equal to or greater than the design discharge and satisfies all the appropriate constraints.
(d) Storm sewers must be placed at a depth that will not be susceptible to frost, drain basements, and allow sufficient cushioning to prevent breakage due to ground surface loading. Therefore, minimum cover depths must be specified.
(e) The sewers are joined at junctions such that the crown elevation of the upstream sewer is no lower than that of the downstream sewer.
(f) To prevent or reduce permanent deposition in the sewers, a minimum permissible flow velocity at design discharge or at barely full-pipe gravity flow is specified. A minimum full-conduit flow velocity of 2 fps is required or recommended by most health departments and is adopted in this study.
(g) To prevent occurrence of scour and other undesirable effects of high velocity flow, a maximum permissible flow velocity is also specified. The most commonly used value is 10 fps and is adopted here.
(h) At any junction or manhole downstream sewer cannot be smaller than any of the upstream sewers at that junction.

Furthermore, the following additional assumptions are made:

(a) The sewer system is a dendritic network converging towards downstream without closed loops.
(b) The sewer system consist of junctions or manholes (nodes) joined by sewers (links). For the sake of simplicity and to demonstrate the models, other facilities such as weirs, regulators, interceptors, etc. are not considered.

TABLE 1. Illinois Least-Cost Sewer System Design Models

Model	Design	Optimization Technique	Hydraulics	Considering Risks	Input
ILSD-1	Sewer diam, crown elevations, manhole depths	DDDP	Hydrograph time lag and Manning's formula	No	Sewer layout, ground elevations, min soil cover, acceptable max and min velocities, cost functions, time and space increments for routing computations, optimization parameters
ILSD-2	Sewer diam, crown elevations, manhole depths	DDDP	Hydrograph time lag and Manning's formula	Yes	Same as above, in addition, design service life, risk-safety factor relationship
ILSD-3	Sewer layout, sewer diam, crown elevations, manhole depths	DDDP and set partitioning	Hydrograph time lag and Manning's formula	No	Manhole locations, ground elevations, min soil cover, acceptable max and min velocities, cost functions, time and space increments for routing computations, optimization parameters

(c) No negative slope is allowed for any sewers in the dendritic network.

(d) The direction of the flow in a sewer is uniquely determined from topographic considerations.

(e) The design inflows into the sewer system are the inlet hydrographs.

(f) A set of simple cost functions proposed by Alan M. Voorhees & Assoc.[1,8] are adopted for illustrative purposes.

OPTIMIZATION TECHNIQUES

Isonodal Line Representation of Manholes

For all the three design models discussed in this paper, the locations of the manholes must be predetermined and is input data for the design. Imaginary lines called isonodal lines (INL) are used to divide the dendritic sewer system into stages. An INL of a given stage passes through all the nodes (manholes) which are separated from the sewer system outlet by the same number of links (sewers). For the purpose of optimization a stage n includes all the sewers connecting upstream manholes on INL n and downstream manhole on INL n+1. As an example, the INL's for an example system used in ASCE Manual 37[2] is shown in Fig. 1. When the sewer layout is specified, the links between the manholes for different stages are known. If the layout is also to be designed, all the feasible manhole connections should be considered.

Discrete Differential Dynamic Programming (DDDP)

For each possible connection of manholes there are many possible sewer slopes and corresponding diameters which could carry the design discharge, although only one of these gives the least-cost system. However, the slope is equal to the difference of crown elevations between the ends of the sewer divided by its length, and the diameter can be determined from the slope and discharge. Hence, the crown elevation at each end of the sewer is chosen as the optimization variable. The objective is to select the set of upstream and downstream crown elevations, among the many possible crown elevations (states) as shown in Fig. 2, that gives the least-cost sewer system. Although standard dynamic programming could be used as the search technique, DDDP has been found[8] far superior for such optimization problems and therefore is adopted. DDDP is an iterative technique for which a trial set of crown elevations for the entire system (called the initial trial trajectory) is first selected together with a range of crown elevations (called corridors) within the state-stage domain (feasible crown elevations). The recursive equation of DP is then used within a corridor to search for an improved trajectory within the corridor. Subsequently, the improved trajectory is used to set up the new corridor for the next iteration. This procedure is repeated until a least-cost design is obtained within an acceptable cost error. Details of DDDP applied to sewer design have been presented elsewhere[6,7,8,12] and hence not repeated here.

MODEL ILSD-1

The Illinois Least-Cost Sewer System Design Model 1 (Model ILSD-1) is the simplest among the three models introduced in this paper. In this model the design involves the determination of the crown elevations, and consequently the slope, diameter of the sewers, and the depth of the manholes. The sewer system layout is predetermined and serves as input into the model. Risks are not considered in the design. DDDP is applied to select the least-cost sewer system. The sewer diameter, d in ft, is computed by using Manning's formula assuming just-full gravity flow

$$d = (4.66 \frac{n^2}{S_o} Q_p^2)^{3/4} \qquad (1)$$

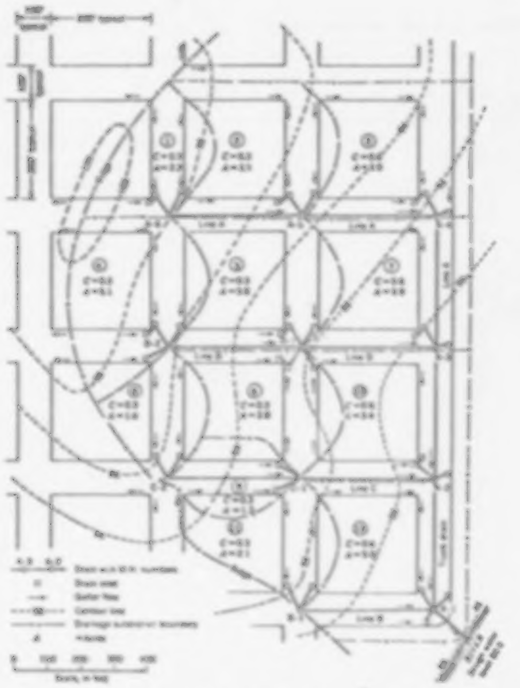
in which n is Manning's roughness factor; S_o is the sewer slope; and Q_p is the peak discharge in cfs of the sewer inflow hydrograph. The sewer outflow hydrograph is obtained through lagging the inflow hydrograph by a travel time, t_f, computed as

$$t_f = L/V \qquad (2)$$

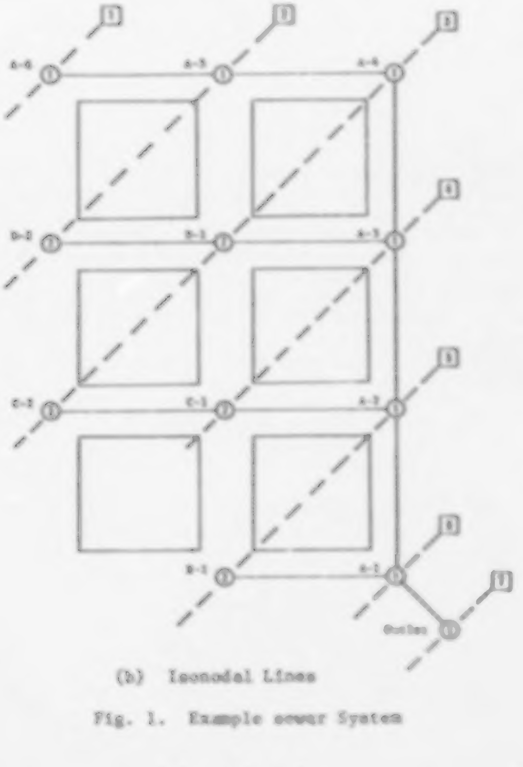
in which L is the sewer length and V is a velocity computed by

$$V = \frac{4\,Q_p}{\pi\, d^2} \qquad (3)$$

The manhole junction condition is described by the principle of mass conservation



(a) Street System Layout[2]



(b) Isonodal Lines

Fig. 1. Example sewer System

$$\Sigma Q_{in} + Q_j = Q_{out} \tag{4}$$

in which Q_{in} is the discharge of the inflowing sewers into the manhole; Q_j is the surface inflow at the manhole, and Q_{out} is the outflow from the manhole into the downstream sewer. Yen and Sevuk[10] have shown that this simple routing method produces hydraulic sewer designs very similar to those obtained by using more sophisticated routing methods. Therefore, this hydrograph time lag method is adopted for all three models because of its simplicity and relatively small computer requirements. The flow charts and computer program listing for Model ILSD-1 can be found in Yen et al.[12]

MODEL ILSD-2

Model ILSD-2 is the Illinois Least-Cost Sewer System Design Model with risk considerations. Risks are considered in the design through the use of a set of risk-safety factor curves for the drainage basin considered. The development of the risk-safety factor curves for a basin has been described elsewhere.[9,11,12]

In the least-cost design considering risks, the cost consists of the sum of the installation cost of sewers and manholes and the expected damage cost during the service period of the sewer. The latter cost is evaluated as the product of the assessed damage value in the event of a flood exceeding the sewer capacity, Q_c, and the risk, i.e., the probability of occurrence of this event during the service period of the sewer. To evaluate the risk, the safety factor is first computed by $SF = Q_c/Q_p$ where

$$Q_c = \frac{0.463}{n} d^{8/3} S_o^{1/2} \tag{5}$$

With the value of SF known, the corresponding risk can be obtained from the risk-safety factor curve corresponding to the service life of the sewer.

Model ILSD-2 is essentially Model ILSD-1 with the addition of risk considerations. The same hydraulic method is used and the sewer system layout is predetermined. Details and flow charts for Model ILSD-2 can be found in Yen et al.[12]

MODEL ILSD-3

Model ILSD-3 is the Illinois Model for Least-Cost Sewer System Design including Layout. This is a screening model based upon DDDP. In addition, the model consists of a scheme (using set-partitioning) to select the least-cost connection of manholes. The sewer system input includes the locations of the manholes and ground elevations and the design gives the sewer layout in addition to the crown elevations, slope, and diameter of the sewers and depth of manholes as for the previous two models. The same hydraulic method is used as in the previous two models. Risks are not considered in the design. Details on the optimization technique have been presented by Mays.[6]

DESIGN EXAMPLE

Many sewer engineers are familiar with the example sewer system used in ASCE Manual 37[2] demonstrating the design of sewer diameters for a given network layout and slopes using the traditional rational method. Hence this sewer system (Fig. 1a) is adopted here as an example to illustrate the advantages of the proposed least-cost design models over the traditional hydraulic design methods.

In ASCE Manual 37 the inflow data were given only as peak flows obtained by using the rational formula. These peak flow data are converted into manhole inflow

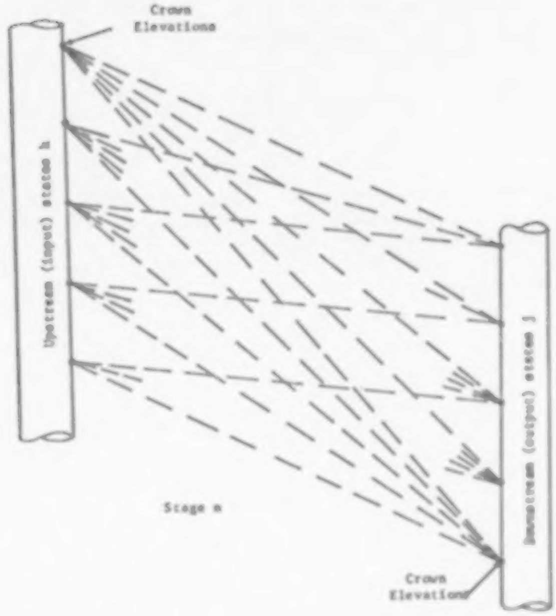


Fig. 2. Drops in Crown Elevations Between Manholes

hydrographs. The inflow hydrographs are assumed to be symmetric and triangular in shape with a base time of 40 min starting at the same initial rise time and with a constant base flow of 0.10 cfs. The peak discharges are listed in Table 2. The minimum sewer size used is 12 in. and Manning's n is 0.013 for all the sewers. The minimum soil cover depth is 3.5 ft.

TABLE 2. Design Example Input Data

Isonodal Line	Manhole Number	Ground Elev. ft	Down-stream Manhole Number	Sewer Length ft	Peak Inflow Q_p cfs
1	1	98.6	1	400	2.0
2	1	94.9	1	400	3.1
	2	96.2	2	400	4.7
3	1	91.8	1	400	6.6
	2	92.3	1	400	1.2
	3	94.6	2	400	1.5
4	1	89.7	1	400	10.1
	2	92.7	1	400	1.0
5	1	89.5	1	400	5.0
	2	91.6	1	400	2.0
6	1	88.5	1	125	7.1
7	1	88.0			

Models ILSD-1 and ILSD-2 are applied to the example system and the resulting sewer diameters, slopes, and crown elevations of the least-cost designs are summarized in Table 3. In applying Model ILSD-2, a 5-yr risk-safety factor curve developed for Urbana, Illinois is assumed applicable and the assessed damage value is assumed to be $10,000 for each of the sewers. The traditional rational method design given in ASCE Manual 37 is also summarized in Table 3 for comparison. The risks associated with these designs over a 5-yr period are listed in Table 3 and the costs are given in Table 4 for comparison. For the ILSD-1 and ASCE designs, the risks are evaluated by using the same 5-yr risk-safety factor curve employed in Model ILSD-2. The safety factor for a sewer is computed by $SF = Q_c/Q_p$ with Q_c given by Eq. 5. Accordingly the risk for the sewer associated with the design can be determined. The expected damage cost for each sewer is evaluated as the product of the risk and the assessed damage value. The expected damage cost computed for the entire system as well as the installation and total costs for the ILSD-1, ILSD-2, and ASCE designs are given in Table 4.

TABLE 3. Designs of Example Sewer System

Upstream Isonodal Line	Up-stream Manhole	Crown Elevations Up-stream ft	Crown Elevations Down-stream ft	Sewer Slope	Sewer Dia-meter in.	Risk
		Design Using Model ILSD-1				
6	1	83.75	83.00	0.00600	36	0.283
5	1	84.69	83.75	0.00234	36	0.592
	2	88.10	85.00	0.00775	12	0.077
4	1	86.20	84.69	0.00378	30	0.610
	2	89.20	86.00	0.00800	12	0.142
3	1	88.30	86.20	0.00525	21	0.554
	2	88.80	86.20	0.00650	18	0.125
	3	91.10	89.20	0.00475	12	0.051
2	1	91.40	88.30	0.00775	15	0.416
	2	92.70	88.80	0.00975	15	0.217
1	1	94.90	91.40	0.00875	12	0.051
					average	0.283
		Design Using Model ILSD-2				
6	1	84.13	83.00	0.00900	42	0.002
5	1	85.44	84.19	0.00312	42	0.036
	2	88.10	84.13	0.00994	12	0.032
4	1	86.20	85.44	0.00191	42	0.046
	2	89.20	85.44	0.00941	12	0.086
3	1	88.30	86.20	0.00525	24	0.113
	2	88.80	86.20	0.00650	18	0.115
	3	91.10	89.20	0.00475	12	0.051
2	1	91.40	88.30	0.00775	18	0.020
	2	92.70	88.80	0.00975	18	0.007
1	1	94.90	91.40	0.00875	12	0.050
					average	0.051
		Design Given in ASCE Manual 37				
6	1	83.55	83.05	0.0040	36	0.670
5	1	85.15	83.55	0.0040	36	0.453
	2	85.15	81.55	0.0090	12	0.066
4	1	86.25	85.05	0.0040	30	0.685
	2	86.75	83.15	0.0090	12	0.249
3	1	87.90	90.30	0.0060	21	0.572
	2	88.05	86.55	0.0070	18	0.145
	3	89.55	86.75	0.0070	12	0.020
2	1	91.00	87.40	0.0090	15	0.451
	2	91.80	87.80	0.0100	15	0.228
1	1	94.35	90.75	0.0090	12	0.066
					average	0.328

As seen from Table 4, applying optimization indeed produces designs with lower costs, and Table 3 further shows that the risk of failure is also reduces, e.g., from 0.328 for ASCE design to 0.283 for Model ILSD-1. The installation cost of the ILSD-1 design is 4% lower than the ASCE design. In fact, by merely adding the peak discharges successively in the network gives the same design discharges as for the ASCE design and a DDDP optimization design for these discharges[12] reduces the installation cost from $70,087 to $69,062.

The superiority of Model ILSD-2 is clearly demonstrated in Table 4. The total cost of this design is 25% lower than that of the ASCE design for a 5-yr service period, and the savings will be considerably more for a longer service period. In order to offset the expected damage costs due to flooding, the sewer sizes are larger than those for the ILSD-1 and ASCE designs (Table 3), providing a better trade-off between installation and damage costs to give a minimum total cost. With larger sewer sizes for the ILSD-2 design, the associated risks are reduced considerably as shown in Table 3.

TABLE 4. Cost Comparison for Example Designs

Model	Cost in Dollars		
	Installation	Damage	Total
ASCE	70,087	(36,037)	(106,124)
ILSD-1	67,001	(31,183)	(98,184)
ILSD-2	76,155	5,602	81,757

CONCLUSIONS

Considerable savings in sewer designs can be achieved by considering the sewers as a system and searching for the least-cost design using optimization techniques. Considering the uncertainties and risks in the design through evaluation of risk-based expected damage costs provides further improvement. In this paper three such least-cost design models are briefly described. Crown elevations and slopes of sewers in addition to their diameters are all determined in the design procedure. In addition, the least-cost sewer layout can also be determined if desirable by using the appropriate model.

ACKNOWLEDGMENT

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THE USE OF LITHIUM CHLORIDE
FOR AERATION TANK PERFORMANCE ANALYSIS

*Robert C. Ahlert
Professor, Chemical &
Biochemical Engineering
Rutgers University

Thomas J. Olenik
Assistant Professor
Civil and Environmental Engineering
New Jersey Institute of Technology

Robert Gesumaria
Graduate Student
Rutgers University

Abstract

Lithium Chloride (LiCl) was used as a tracer to analyze the flow-through performance of a mechanical and diffused aeration process at two different activated sludge plants. A slug of aqueous LiCl was dumped at the entrance of each tank and effluent samples were anlayzed using an atomic absorption spectrophotometer. These results and the corresponding mathematical models showed how the existing facilities were operating in an inefficient manner. It is reasonable to assume that this technqiue can be applied to all aeration tanks with the hope of eliminating dead space and shortcircuiting.

Introduction

The design of aeration tanks for the activated sludge process revolves around several basic design parameters. These parameters are: biochemical oxygen demand (BOD) loading, detention time in the tank, mixed liquor suspended solids (MLSS), sludge age etc.. All of these design values are supposed to guarantee sufficient destruction of waste products in order for the sewage treatment plant (STP) to achieve its design removals of BOD and suspended solids. After construction of the facilities, there is seldom any checking of aeration tank performance unless removals are not being met or operational problems appear. However, it is entirely possible that an adequately designed aeration tank may be operting at very inefficient levels with regard to the flow of the mixed liquor through the tank's volume. That is, short-circuiting, existence of dead space or a combination of the two may be occuring that result in less than ideal tank performance.

A check of the flow-through conditions by use of a tracer will indicate the existing conditions. Based on this analysis, which is described below, it may be possible that an existing aeration tank can accept a higher loading in the form of flow and/or waste. Therefore, by performing this analysis a municipality may be able to avoid unnecessary expansion of its aeration tank system or the plant may be able to accept additional flow.

Lithium Chloride Tracer Analysis

Lithium Chloride as a Tracer

One of the previous drawbacks of tracer analysis of aeration tanks was the poor performance of the tracer used. That is, organic dyes are subjected to biological breakdown along with incorporation of the dye into the sludge particle resulting in inaccurate test results. In the studies described below, it was decided to use lithium chloride (LiCl) as the tracer for the following reasons:

1. LiCl is highly soluble in small amounts of water.
2. The LiCl will not be incorporated into the sludge particles.
3. The concentration of the Li can be detected accurately to 0.01 milligrams per liter (mg/l) by an atomic adsorption spectrophotometer (AAS).
4. LiCl is fairly inexpensive (approx. $1.20/lb.).

Analysis of Tracer Testing

As outlined in Himmelblau and Bischoff's (2) work on Population-Balance Models, a vessel whether it is for a chemical or biological reaction, can be described through the use of age distribution functions. Most chemical and biological reactors have been studied under the assumption that their flow patterns are either plug flow or perfectly mixed. Plug flow can be defined as that flow in which the fluid velocity is uniform over the entire cross-section of the vessel (fluid particles do not intermingle with other fluid elements). Perfect mixing assumes that the tank's contents are completely homogeneous (effluent properties are identical to the tank's properties). In actual reactor performance, the flow patterns lie between these two extremes. In order to describe what is occuring within the tank and, in turn, achieve a description of the effluent's characteristic, an age distribution function is developed through use of a tracer or other tracking mechanism. Therefore, a graph of lithium concentration versus time is developed by sampling the effluent end of an aeration tank. This graph can then be compared to the one shown as Figure 1. The bell-shaped curve in this figure is what is expected for actual reactors. The other curve exhibits dead space (long tail) and some short-circuiting (peak to the left of $\bar{t}$ or average detention time).

Mathematical modeling of biological reactors such as aeration tanks and receiving waters has been studied with great intensity over the last decade. These models often attempt to describe the ability of the reactor to remove BOD, etc., by obtaining a large amount of field data and applying it to the model. Recently, a method based on the "black-box" approach developed by Wilson and Norman (3) has been attempted. Very simply this method uses a network of ideal well-stirred tank and plug flow reactors, to fit residence time distribution data from either laboratory scale models or field tracer studies. Thus, this input-output method allows all of the complex internal processes (turbulence, etc.) to be reflected directly in the network without monitoring all of the interior and often quite complex processes. The network model will not of necessity take the same physical appearance as the natural system. But the great advantage of including micro-mixing processes and stochastic variations greatly affect the lack of direct physical correspondence to the actual reactor. This method of using combined plug flow and well-stirred reactors can be of great value when describing the partially mixed reactors that occur in treatment plant or in the environment. The model can be used to predict the effect changes in a system, such as loadings, may have on the reactor unit process or a receiving water.

The modeling techniques that were used are those based on Wilson's work (3) and a recent paper by Ahlert and Hsueh (1) of the Department of Chemical and Biochemical Engineering at Rutgers University. Mr. Hsueh was especially helpful in setting up the program and analyzing the data.

Wilson utilized the "black-box" approach and the basic concepts of the Fourier Transform Function. That is, by ignoring the complex internal mechanics of a unit process, the problem of data collection involved in a deterministic type model is avoided. The Fourier Transform Function or Laplace Transform allows transfer of time domain data collected at the effluent end of a tank into the frequency of or domain. This action yields a description of the system by algebraic relationships in the frequency domain instead of complicated linear differential equations in time domain. This change allows the use of block diagrams to describe the process with a model that can predict what will happen to the system when loaded differently.

The transfer function is defined by the equation:

$$Z(s) = \frac{Y(s)}{X(s)} \qquad (1)$$

where Z(s) is the transfer function, Y(s) and X(s) are the Laplace Transform of the output and input data respectively. Therefore, once Z(s) is known for a system, any other applied loading in terms of X(s) can be converted to output in the frequency domain and the characteristic equation of the output in the time domain (y(t)) by performing the inverse transform operations.

The transfer function and the inverse computations are relatively easy to perform. This fact is applied in using Wilson's approach, as the lithium chloride was inputed as a Dirac-delta function. The equations and assumptions involved in Wilson's method are described below:

The frequency content S(ω) of an aperiodic function is described by its Fourier Transform

$$S(\omega) = F(f(t)) = \int_{-\infty}^{\infty} f(t)\, e^{-j\omega t}\, dt \qquad (2)$$

where

$$j = \sqrt{-1} \quad \text{and} \quad j\omega = s$$

For convenience purposes, S(ω) is normalized by dividing it by the value at zero frequency.

$$S(\omega)_n = \frac{F(f(t))}{\text{Area under } f(t)} \qquad (3)$$

then the Fourier Transfer Function is given by

$$Z(\omega) = \frac{\int_o^{T_y} y(t)\, e^{-j\omega t}\, dt}{\int_o^{T_x} x(t)\, e^{-j\omega t}\, dt} \qquad (4)$$

where T_y and T_x are the upper limits of the integration for the output and input function, respectively, and x(t) and y(t) are the time domain functions of the input and output signals respectively. By applying the identity

$$e^{-j\omega t} = \cos \omega t - j \sin\omega t \qquad (5)$$

the real, Re(ω), and imagining, Im(ω), parts of the Transfer Function are given as:

$$Re(\omega) = \frac{AC + BD}{C^2 + D^2} \qquad (6)$$

$$Im(\omega) = \frac{AD - BC}{C^2 + D^2} \qquad (7)$$

where

$$A = \int_o^{T_y} y(t) \cos(\omega t)\, dt \qquad (8)$$

$$B = \int_o^{T_y} y(t) \sin(\omega t)\, dt \qquad (9)$$

$$C = \int_o^{T_x} x(t) \cos(\omega t)\, dt \qquad (10)$$

$$D = \int_o^{T_x} x(t) \sin(\omega t)\, dt \qquad (11)$$

The model block diagram construction can start based on two ideal chemical reactors. The two reactors are the plug-flow tubular reactor (PFTR) which acts as a pure time delay mechanism, and the continuous stirred tank reactor (CSTR) which is an instantaneously mixed system where dispersion reaches a maximum. The PFTR and CSTR are linear in the time domain and are transferred into the complex (s)-domain to obtain the system Transfer Functions. Linearity allows the construction of complex networks based on these components.

Taking the field data, Equation 5 through 11 are used to derive the real and imaginary parts of the transfer function. A Bode plot is used in defining poles and zeros; from these a first estimate of the number of CSTR components needed can be made for a trial network configuration. The network configurations are evaluated by a least-squares procedure by using the sum of the squared vectorial deviations in the frequency domain as shown below in Equation 12.

$$\Phi = \frac{1}{n} \sum^{\omega=\omega_{max}} (Re(\omega)_o - (Re(\omega))_p^2$$

$$+ (Im(\omega)_o - (Im(\omega)_p^2 \qquad (12)$$

where the o and p refer to observed data and predicted values using the model, respectively.

Tests Performed and Results

The techniques described were used at two activated sludge plants, the Madison-Chatham and Hanover Park sewage treatment plants.

Madison-Chatham Plant

The aeration system at the Madison-Chatham plant is divided into two physically distinct tanks. The first and largest tank is a diffused air system. The other tank, containing mechanical aerators, was the one chosen to be traced using lithium chloride (Figure 2). The equipment employed was the following:

1. 50 lbs. of LiCl.
2. 2 Sigmamotor automatic samplers.
3. Garbage can.
4. 10 feet of 6-inch smoke pipe to dispense the solution of LiCl.

The test procedure was to dump instantly a slug of aqueous LiCl solution, by use of the garbage can, into the influent pipe of the mechanical aeration system. An instantaneous slug was necessary to approximate a Dirac-delta function to make the mathematical model of the system easier to produce. Automatic samplers (Sigmamotor Co.) were needed to obtain samples on a continuous basis after the LiCl had been dumped. These samplers can be set at time intervals ranging from 1 to 60 minutes. At the end of each sample period the machine resets itself to another bottle, so discrete, not combined samples are taken. Through use of an automatic purping device, the sample pump and tubing are evacuated. Two samplers were needed because of recycling of secondary settling tank sludge that could contain some lithium and return it to the system. Two samplers were located as shown in Figure 2, and were in operation for about 72 hours. Samples were analyzed using an atomic adsorption spectophotometer (Perkins-Elmer Model No. 403).

The data are plotted using concentration versus time as the scales in Figure 3. A computation of the mass balance for lithium showed that 88 percent of the lithium was accounted for. Since this first run operated at sample time intervals of 30, 40 and 60 minutes, and since it was felt that a great deal of short-circuiting occurred in the first 30 minutes, the first 3 hours of the experiment was repeated using 35 pounds of LiCl. The time interval of the sampling for the second run was 1 minute for the first half hour and 5 minutes to the end of the experiment (4 hours total). A mass balance showed that 20 percent of the lithium was accounted for in this time period (Figure 4).

The curve of concentration versus time for the first run as shown in Figure 3 can be compared to Figure 1. This curve shows that appreciable amounts of tracer still exist in the aeration tank well past the average detention time of about 5.3 hours (design detention time is 4.5 hours). Also, during the first run (50 pounds of LiCl) periodic samples of the dead spots (see Figure 5) showed higher concentration of lithium when compared to the effluent suggesting these dead spots were isolated areas where detention time of the mixed liquor is higher. It should be noted that the return sludge, did not contribute appreciable amounts of lithium because the sludge had been diluted considerably by flow from the much larger diffused aeration tanks.

From the above experimental results it can be seen that the hydraulic flow through characteristics of this aeration tank causes a severe short-circuiting and a limited amount of dead space. It is obvious that this tank is not being used in an efficent manner. This fact is brought out further by an examination of the mathematical models produced for the two runs described above. An examination of Figures 6 and 7 that were developed through the use of a computer program allows the following additional conclusions:

1. The optimum models obtained for each run and their transfer functions can now be used to predict the performance of the aeration tank for various loadings.

2. The second run is an improvement over the first, because of the fact that the second run's data were taken at a smaller time interval. From Figure 7, the small effect short-circuiting (segment f_2"f_1') has on the overall model can be seen. The bottom half of the model (segment f_2') is where 95 percent of the flow passes through, which results in a large increase in the residence time. Thus, the summation of the residence times (T_3, T_4, and T_5) adds up to approximately 380 minutes (6.3 hours) which exceeds the average design detention time of 4.5 hours. It is felt that the poor hydraulics of the system causes this effect.

Florham Park Plant

This plant was chosen to be tested in a similar fashion because of the fact that its method of aeration was by diffusers. A flow diagram is shown below (Figure 8).

The same procedure used at the Madison-Chatham Plant was applied at this plant. The actual results are shown in Figures 9 and 10 with the following observations made:

1. An actual average detention time of 8.56 hours was observed (Figure 9) as compared to the design detention time of 4 to 6 hours.

2. On a mass basis, 89.5 percent of the Li was recovered in 30 hours of sampling.

3. Branch f_1 (0.76Q) shows a large amount of dead space in the system. The detention time in this branch ($T_1 + T_3$) is 12.37 hours (742.42 minutes). This value greatly exceeds the design detention time of 4 to 6 hours which is computed by the ratio of tank volume to flowrate. Branch f_2 (0.24Q) shows a significant amount of short-circuiting in the system. The detention time in this branch ($T_2 + T_2 + T_3$) is 2.05 hours (123.12 minutes) which is considerably less than the design detention time of 4 to 6 hours cited above.

Conclusions and Recommendations

It appears obvious from the two studies performed concerning aeration tanks used in the activated sludge process, that poor flow-through conditions cause a gross inefficiency in the treatment plant system. While this technique can produce a very involved and costly analysis if the modeling is performed, a simple concentration of Li versus time can give an engineer an adequate picture of what is occurring in the aeration tank that is the key unit process in the treatment plant. This is not limited to the analysis of aeration tanks. It is hoped that this technique will be applied to receiving water analysis along with expanded uses in analyzing existing sewage treatment processes.

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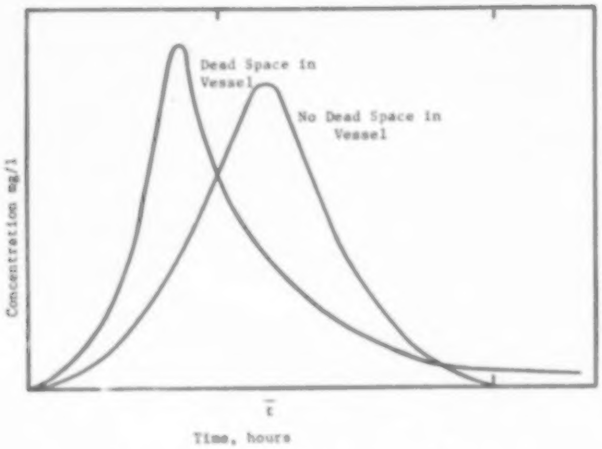
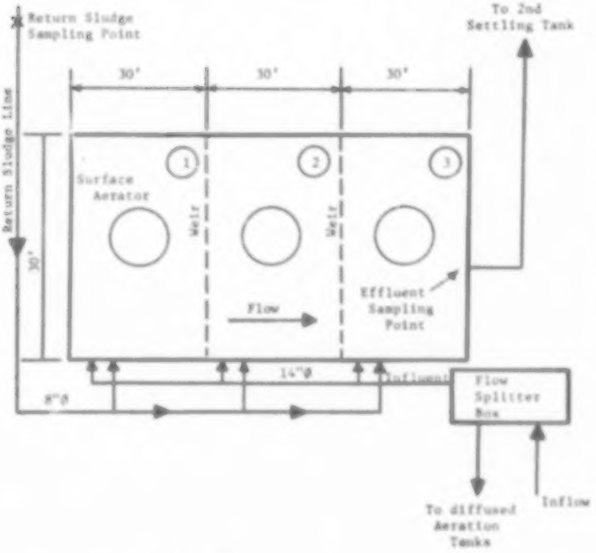


FIGURE 1 IDENTIFICATION OF INEFFICIENT AERATION TANK OPERATION


Return Sludge Sampling Point
To 2nd Settling Tank
30'
30'
30'
Return Sludge Line
30'
1
2
3
Surface Aerator
Weir
Weir
Flow
Effluent Sampling Point
14"Ø
Influent
8"Ø
Flow Splitter Box
To diffused Aeration Tanks
Inflow

Tank Numbers	Depth feet	Volume $feet^3$	Volume Gallons
1	10	9,000	67,320
2	10	9,000	67,320
3	14	12,600	94,248

FIGURE 2 MECHANICAL AERATION SYSTEM, MADISON-CHATHAM PLANT

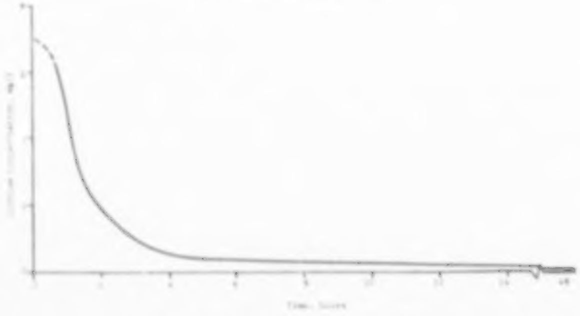


FIGURE 3 LITHIUM TRACER STUDY, FIRST RUN, MADISON-CHATHAM PLANT MECHANICAL AERATION SYSTEM

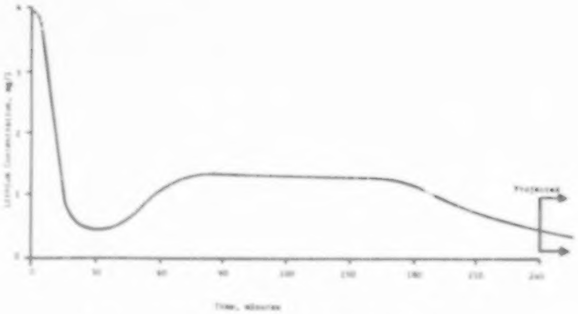


FIGURE 4 LITHIUM TRACER STUDY, SECOND RUN, MADISON-CHATHAM PLANT MECHANICAL AERATION SYSTEM

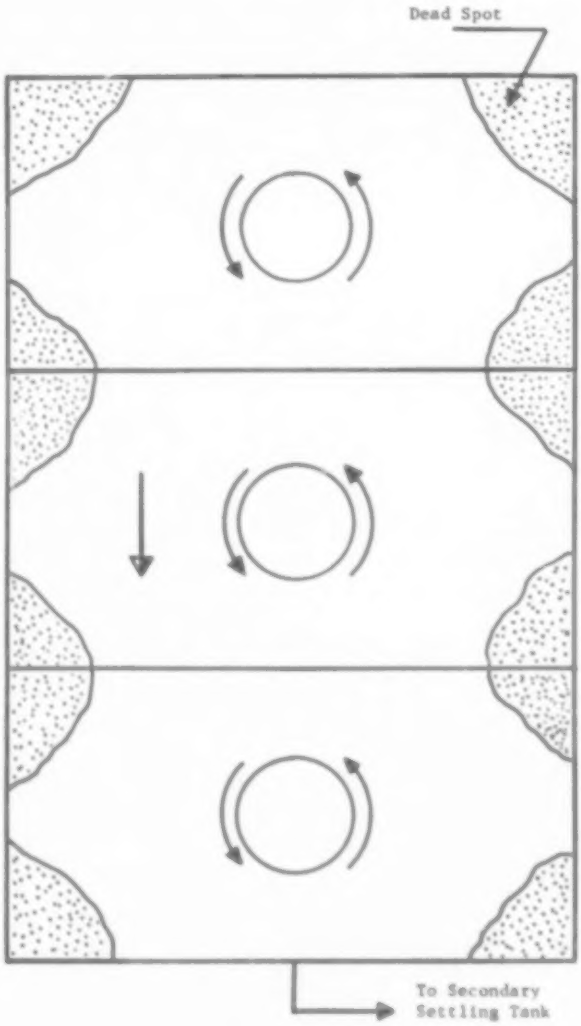
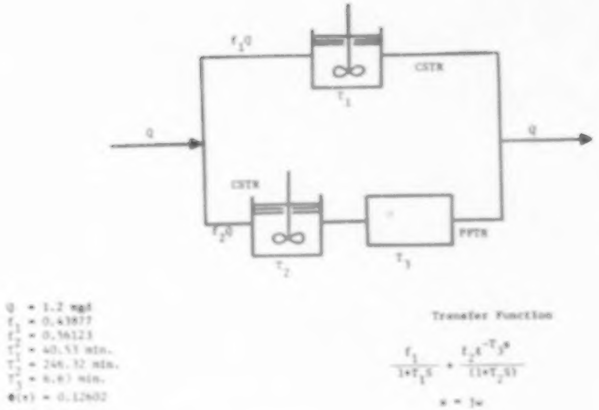

Dead Spot
To Secondary Settling Tank

FIGURE 5 PLAN VIEW OF MECHANICAL AERATION TANK SHOWING LOCATION OF DEAD SPOTS


f$_1$Q
CSTR
T$_1$
Q
Q
CSTR
f$_2$Q
PFTR
T$_2$
T$_3$
Q = 1.2 mgd
f$_1$ = 0.43877
f$_2$ = 0.56123
T$_1$ = 40.53 min.
T$_2$ = 246.32 min.
T$_3$ = 6.63 min.
Φ(ε) = 0.12602
Transfer Function
s = jw

$$\frac{f_1}{1+T_1 s} + \frac{f_2 e^{-T_3 s}}{(1+T_2 s)}$$

FIGURE 6 MIXING MODEL FOR RUN NO. 1, MADISON-CHATHAM PLANT MECHANICAL AERATION SYSTEM

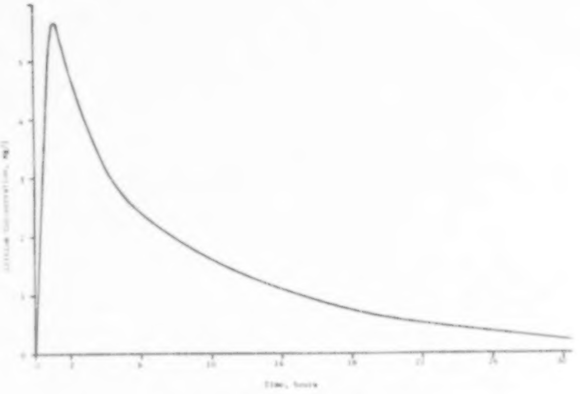


FIGURE 9 LITHIUM CONCENTRATION VERSUS TIME
FLORHAM PARK SEWAGE TREATMENT PLANT,
FLORHAM PARK, NEW JERSEY
DIFFUSED AERATION SYSTEM

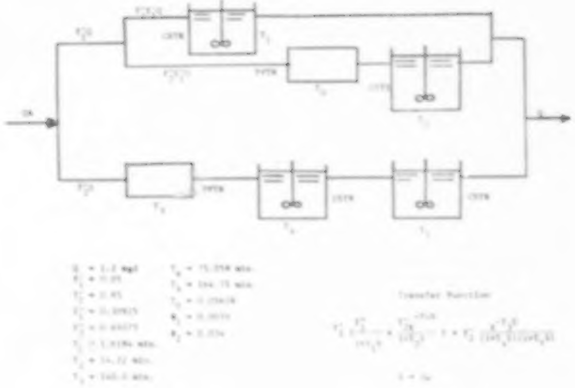

f$_1$Q
CSTR
T$_1$
PFTR
CSTR
Q
f$_2$Q
PFTR
CSTR
CSTR
Q = 1.2 mgd
Transfer Function
s = jw

FIGURE 7 MIXING MODEL FOR RUN NO. 2, MADISON-CHATHAM PLANT MECHANICAL AERATION TANK

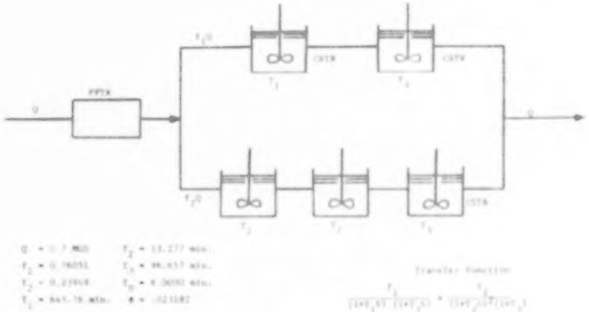

f$_1$Q
PFTR
CSTR
CSTR
T$_1$
Q
Q
f$_2$Q
CSTR
Q = 0.7 MGD
f$_1$ = 0.76051
f$_2$ = 0.23949
T$_1$ = 641.76 min.
T$_2$ = 13.277 min.
T$_3$ = 96.637 min.
T$_0$ = 8.3050 min.
Transfer Function

FIGURE 10 REACTOR NETWORK CONFIGURATION, DIFFUSED AERATION SYSTEM
FLORHAM PARK SEWAGE TREATMENT PLANT
FLORHAM PARK, NEW JERSEY

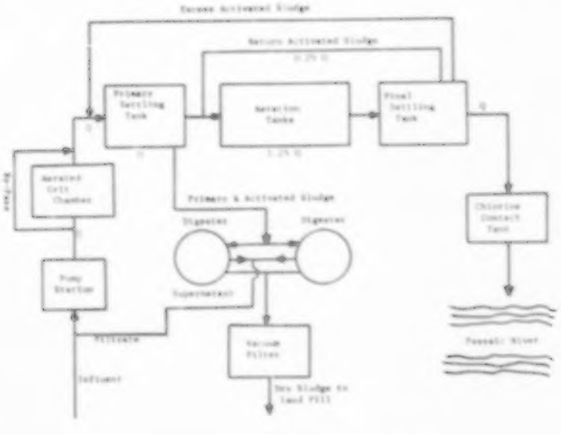

Excess Activated Sludge
Return Activated Sludge
Primary Settling Tank
Aeration Tanks
Final Settling Tank
Q
Aerated Grit Chamber
By-Pass
Primary & Activated Sludge
Digester
Digester
Supernatant
Chlorine Contact Tank
Pump Station
Filtrate
Vacuum Filter
Influent
Dry Sludge to Land Fill
Passaic River

FIGURE 8 FLOW DIAGRAM OF THE FLORHAM PARK SEWAGE TREATMENT PLANT, FLORHAM PARK, NEW JERSEY

SWAN

A SEWER ANALYSIS AND MODELING SYSTEM

Elias C. Tonias, P.E.
Director of Computing Center and Associate

Philip C. King, P.E.
Project Engineer

ERDMAN, ANTHONY, ASSOCIATES, CONSULTING ENGINEERS, ROCHESTER, NEW YORK

ABSTRACT

The need for a thorough understanding of the sewage collection systems for many municipalities has resulted in the development of a system of computer programs to analyze an existing network. This computer system, called SWAN (an acronym for Sewer Analysis), can be employed to examine the collection network as a whole or in part(s), thus enabling the investigators to see the total character of the network at a glance and to make coordinated decisions concerning expansion and improvement.

SWAN can store an entire sewage collection network on a data base which can be easily modified and employs a mathematical model to simulate the network flows under various sanitary and storm conditions and combinations thereof. SWAN was originally based on the Rational Method. Recent modifications have incorporated the Surface Hydrograph Method commonly referred to as the Chicago Method.

Although SWAN's primary purpose is to analyze existing sewer systems, it may be utilized as a design tool. The principle of design by iterative analysis is facilitated immensely by SWAN's built-in feature of recommending appropriate pipe sizes for upgrading inadequate sewer reaches. Graphic documents produced automatically by the computer system may be utilized as final report or contract documents.

SWAN is ideally suited for a small (IBM-1130) computer readily available to many consulting engineering offices and small governmental agencies and municipalities. Although SWAN is intended for batch processing, it may easily be revamped for an inter-active environment.

The authors wish to acknowledge the efforts of Mssrs. Charles S. Hodge and Alfred J. DeYoung during the development of the original system.

INTRODUCTION

The original sewer system in many older communities was a storm sewer, as this was the bigger and more visible problem, which evolved into a combined sanitary and storm sewer. In many other communities, it was economics that dictated that the sewers be built as combined sewers. As time went on, community-wide treatment facilities were built. The excessive storm flows necessitated the construction of overflows into any convenient water body. It has become necessary therefore for municipalities to take a very close look at their wastewater collection systems, especially where the collection systems are combined facilities.

The result is a growing need for information about existing sewer networks and the character of the storm flows that are carried in these networks. Too often, a municipality's wastewater collection system is not known and is not inspected unless a problem exists. Existing sewer systems are usually the result of a series of expansions and improvements to the original, and often no longer adequate set of conduits. Urban growth has placed a burden on the older conduits and in many situations the systems have not been improved to handle these additional flows.

This need to understand the sewage collection and transport systems has necessitated the development of numerical techniques for analysis and flow simulation of complex sewer networks. There are presently several computer software packages designed to accomplish this.

When creating a sewer modeling program, the following parameters must be considered:

1. Methodology of load generation
2. Methodology of load transport
3. Special features to be analyzed such as pumps, overflows, weirs, etc.
4. Extent of network to be analyzed (how many pipes, manholes, overflows, or other special features).
5. Ease of use by the practicioner with respect not only to input generation but also to output interpretation.
6. Availability of and selection of hardware

SWAN is an entirely analytic system. It does not employ statistical methods other than those necessary to reduce field observed statistics. SWAN employs common hydraulic principles that are used by hydraulic engineers in normal design and analysis such as Manning's Equation, Hazen-Williams Equation, the Rational Method, the Surface Hydrograph Method (Chicago Method), hydrograph and backwater techniques. SWAN's use is enhanced by its ability to apply them to a large network, thereby relieving the engineer from tedious calculations and allowing him to concentrate on the major questions.

OPERATIONAL CONCEPTS

SWAN receives data and performs operations through a series of commands. These commands are one word signals which transfer control to the various operations which may in turn receive data. Commands may be streamed together. Each command has some terminal device which will cause the system to seek a new command. All of the commands are tied together in that they all use the various files which are developed in a specific order. Therefore, some commands may be prerequisite for others.

Most of the commands employ extensive error diagnostics. There are five basic groups of commands in SWAN:

1. The CONTROL, GEOMETRY and EDIT commands are used to build the data base from which all other operations take their cue.
2. The VELOCITY, GAUGING and FLOWS commands are used to reduce field observations and generate reports for system verification.
3. The PROFILE, CONDITIONS and PLOT commands generate profile plots with a table of conduit descriptions.
4. The LOAD, CURVE, HYDROGRAPH and BACKWATER commands are used to analyze and simulate the flows.
5. There are three other commands: END, STOP and EXIT, which are used to terminate commands or the entire system run.

The prerequisites of SWAN are basic in concept:

1. There must be a problem definition - something to analyze.
2. The system to be analyzed must be described accurately.
3. The user has to be familiar with the actual network and should have an in-the-field awareness of actual conditions.
4. The user must have a knowledge of hydraulics and hydrology.

PROBLEM DEFINITION

The use of SWAN must be pointed towards a specific situation. The user must know what he is attempting to show with his sewer analysis. SWAN is not a mysterious miracle worker. It is a tool to be employed to effectively analyze a problem. In turn, it may be used to assist in designing a correction for the problem.

In order to utilize SWAN, data must be collected and entered into the data base. Sewer networks have to be described by their geometrics. This description of the sewer geometry requires the following information:

1. Length of each conduit between manholes.
2. Shape of conduit and dimensions.
3. Invert elevations at each manhole.
4. Manning's n for each conduit.
5. Continuity of flow.
6. Manhole rim elevation if profile plots are desired.

The geometry is usually available to municipalities in the form of design or as-built plans or previous sewer studies. The definition of the sewer geometrics is fundamental to proper SWAN operation. Should data about existing sewers be questionable, field measurements should be made to resolve these questions. SWAN can analyze systems containing a multiplicity of different basic conduit cross-sections. There are presently 33 shapes on line.

The hard geometric data which defines a sewer must be supplemented by a geometric logic describing the layout of each sewer component. This logic is described by nodes (manhole numbers) and incidences (downstream manhole to upstream manhole). The sewer network has three basic elements: the "reach", the "strip", and the "drainage area". The reach, the smallest and most descriptive element, consists of two manholes and their connecting conduit. Manholes may be real or "pseudo": a real manhole actually exists in the network; the "pseudo" or imaginary manhole is a nodal point at which some feature in the conduit changes. The pseudo manhole provides the system with the flexibility to describe changes in the conduit between manholes. Thus the conduit in each reach is uniform in shape, material and slope.

Many reaches linked end to end would constitute a "strip". A strip begins at some downstream manhole (real or pseudo) and proceeds manhole by manhole to some upstream manhole. This upstream point may be a dead end manhole or it may be the limit of investigation.

Many strips tied together by common manholes would constitute a "drainage area". The drainage area can have only one outlet.

FIELD OBSERVATIONS AND VERIFICATION

The mathematical model of flows in a sewer network built by SWAN is only as good as the data base on which it is founded. Therefore, it is advisable that field observations be made in order to validate the base and subsequent modeling.

Field observations should include determination of Manning's n where necessary, storm flow gauging, dry weather flow gauging, condition of sewer conduits and manholes and resolution of ambiguous geometric data.

The character of drainage areas serviced by a network may change with time, especially in districts close to central business areas. Urbanization results in a general increase in the imperviousness of a watershed, rendering storm or combined sewers in these districts inadequate. Observations of these conditions are extremely important in order to validate the computer model.

Verification of the SWAN modeling may be made by placing flow meters capable of recording the water surface with respect to time at control manholes. By appropriate reduction of recorded data, actual hydrographs for recorded storms may be obtained at each of these test manholes. Theoretical hydrographs for the same points and recorded storms may be generated by SWAN and superimposed upon the actual hydrographs for verification.

HYDROLOGIC CONSIDERATIONS

There are presently several methods available to determine the amount of rainfall entering a sewer network ranging from oversimplified approximations to highly mathematical modeling approximations. All of the available methodologies, regardless of their sophistication, do depend upon empirical data whether they are runoff coefficients, imperviousness factors or impoundment constants. Of these, two have gained widespread use in present practice, the Rational Method and the Surface Hydrograph or Chicago Method.

SWAN was originally designed to determine runoff by the Rational Method. Verification of its results was made for 25 year design storms. Recently the Chicago Method was incorporated into the system to allow the user this option.

SWAN's application of the Rational Method is based on rainfall-intensity curves promulgated by local weather offices utilizing contributing areas of city block size or smaller and composite imperviousness factors. The program uses the inputed time of concentration and the computed elapsed time of flow in the sewer as a storm duration abscissa to find the rainfall intensity from the rainfall/intensity curve. Times of concentration, much like the Manning n factors, require judgment and evaluation. Published tables are available to assist in their selection.

In addition to direct time of concentration entry, SWAN offers the ability to compute such time by the equation:

$$TINLT = 1.8(1.1-BCOF)(BLEN)^{0.50}/(BSLOP)^{0.333}$$

Where: TINLT is the inlet time in minutes
BCOF is the basin coefficient of runoff
BLEN is the basin length in feet
BSLOP is the basin slope in percent

The Rational Method is based on a uniform rainfall on the entire drainage area under investigation. Violent summer storms of infrequent occurrence do not fit this pattern as they are not uniform in rainfall intensity nor uniform on the entire area. Users therefore should be aware of these limitations because they tend to yield conservative results and generally indicate too many conduits as being undersized when such a storm is applied.

SWAN's application of the Chicago Method utilizes a model hyetograph and generates time dependent surface hydrographs for every manhole. These hydrographs take into consideration surface imperviousness and impoundments as well as evaporation.

SYSTEM LOADS

SWAN offers the ability to load the sewer system with domestic and industrial loads, storm flows and infiltration. The storm load determination has been described under the hydrologic considerations of this report. Domestic loads may be defined by acres, population density and per capita usage, census population and per capita usage or direct point load. Infiltration and industrial loads are entered as direct point source loads or as a per capita allowance.

The loading feature (called the LOAD operation) is employed to analyze nearly all situations. It applies the normally accepted design methods in an analysis mode. It indicates those conduits which are undercapacity for the specified condition.

The LOAD operation can be applied directly to analyze proposed sewers. The effect of urbanization of a network's watershed can also be analyzed to indicate the deficiencies or unused capacity of the network. The effect of proposed sewers on an existing network is still another powerful application which can provide insights into land use management under existing conditions.

With sanitary accumulations, combined sewer overflows to receiving waters can have their pollutant quantity predicted for specific storm conditions. Increases in dry weather sanitary flows caused by dramatic changes in the area served by a network may require readjustment of a combined sewer's overflow regulator.

The LOAD command, having received the loads of the manholes, proceeds to accumulate them upstream to downstream keeping track of time of concentration (Rational Method) and elapsed travel time of flow in the sewer.

Having determined the flow, the program institutes a half interval search based upon the continuity of flow and Manning's equations to find the depth of flow. The search starts at one-half the full depth and continues until one of the following acceptance criteria is met:

1. Change in depth from previous trial to present trial less than 0.001 inches.
2. Load flow previously computed differs from flow at trial depth by less than 0.01 cfs.

Once the depth is found, the velocity is easily calculated and the elapsed time of flow is incremented by the time-of-flow in the present reach.

If the flow developed previously is greater than the capacity of the conduit, the search operation is omitted and the time is computed based on full depth of flow. Any reach which had a computed flow greater than capacity is flagged and its description is stored for future tabulation. The command can institute a "design" which will give the size of a circular conduit which will carry the load using a Manning's n of 0.013 and at the slope of the existing sewer.

HYDROGRAPH DEVELOPMENT

Hydrographs of flow from a watershed are useful tools for analysis of any facility carrying or treating storm flow runoffs. While the Rational Method is weak for analysis of runoff, the hydrograph development techniques incorporated into SWAN can be utilized for analysis of any size uniform intensity storm passing in any direction across the watershed area. Hydrographs can be developed for any reach in the drainage area for any given storm. In this application, the physical wave front of the storm flow can be developed and time-flow relationships can be derived and applied to a backwater analysis.

Storm flow hydrographs are powerful devices for analyzing quantity of overflow to receiving waters. SWAN's hydrograph module also provides mass flow diagrams. The developed hydrographs and mass diagrams in the form of coordinates of flow or mass versus time may be printed or plotted.

Sewage treatment of storm water is gaining in popularity. Although it is not new, the treatment of storm water is far from being a well established science. Design criteria are presently being formulated by regulatory agencies. The basic design parameters for storm water treatment are rate and quantity of storm runoff. These parameters are developed by the hydrograph feature of SWAN.

The actual hydrograph development is based on an accumulation of simple trapezoidal hydrographs of each runoff area. For the Rational Method, time of concentration is an important factor. A new element has been added: "start time". For even the most intense storms, rainfall must saturate the ground before runoff begins. Asphalt and concrete pavements have cracks and voids that trap water before runoff begins. This period before water eventually reaches the sewer is called "start time". It can be a matter of seconds or minutes and is a judgment factor as is time of concentration. For the Chicago Method, the above are taken into account in the surface hydrograph generation.

The HYDROGRAPH command accumulates the local watershed hydrographs. It takes its ordinate (either flow or watershed area) and adds to it all the other local hydrographs, displacing each by its travel time down to the reach being investigated. Each of the local watersheds should not exceed an area of about 2 acres. If the areas are larger, the assumption of a trapezoidal local hydrograph becomes questionable.

The hydrograph method can be used to give a reasonable approximation of the effect of a uniform storm on the drainage area but should not be substituted for the actual field observed flows.

The application of a uniform storm to a drainage area is a problem with the hydrograph as it is with the Rational Method in the LOAD command. The difference is that with the HYDROGRAPH command, the input may be selected to conform to an actual storm. Accepted unit hydrograph techniques can be employed by using an intensity of 1.0 to create the unit hydrograph.

BACKWATER

Backwater techniques have long been recognized for the analysis of open channel flow (creeks, rivers, ditches, etc). In a closed conduit the backwater principles are the same except when the sewer is surcharged, i.e. flowing full under a head. Surcharged sewers can be analyzed using pressure flow principles.

The availability of a backwater technique analysis to flow in sewers allows a multitude of applications. The most frequent application is the analysis of a series of reaches having a constriction caused by a singular undercapacity conduit.

The backwater analysis in SWAN can perform two functions:

1. Calculate the required piezometric head to sustain a given flow.
2. Calculate the flow sustained by a predetermined piezometric head.

The first function can be applied to analyze the surcharge capacity of a sewer. This capacity may be significantly larger than the gravity flow capacity. The surcharge capacity of a sewer is important when sewers are analyzed for short-term high-intensity storms. This type of storm has been historically ignored because of the complex nature of any manual analysis. Runoff flows through the sewer in a time-related manner, i.e. the peak flow, need be sustained for only a short period of time (say 3 to 5 minutes). This peak may be 25% to 50% greater than the gravity flow capacity. The sewer can in many cases carry this flow. It has been shown that a storm sewer that was designed for a 10 year recurrence-period-rational-method storm can sustain a 25 year high-intensity short-term storm. The analysis of these storms is a difficult process and requires the development of hydrographs for specific storms.

The ability to calculate a flow sustained by a given head is useful in determining surcharged flows for specific upstream conditions in a sewer. Flow splitting caused by overflow regulators or relief sewers is a good example. Overflow regulators are usually designed in a gravity flow environment. However, in actual practice, these regulators may be surcharged during peak flows, especially if they are regulating flows from dense urban areas.

The operation must start at a known elevation at the downstream end of the investigation. In a sewer this could be one of two conditions.

1. The water surface elevation of a receiving water if the outfall conduit is submerged.
2. The known starting elevation as a function of the conduit hydraulic properties if the sewer flow falls free such as in a drop manhole device or in an overflow outfall.

Using the starting elevation, the operation applies "gradually varying flow" theory to find the water surface within a reach up to its upstream manhole. Using the conservation of energy principle, the starting elevation for the next reach can be calculated. This procedure is repeated until the limit of investigation is reached.

Gradually varying flow theory considers that the water surface can be predicted by a profile curve. This profile is a function of the quantity of flow and the geometrics of the channel.

The flows utilized by the BACKWATER command may be defined in one of three manners.

1. Direct Q (flows in cfs) at each manhole.
2. Flows in terms A*C with a request for a half interval iteration search to determine the flow and subsequent water surface elevation (piezometric head).
3. A modification of 1 above, where Q's are read from the surface runoff hydrographs (Chicago Method) computed earlier in the system and stored in a file.

The third type of loading above may be explained by Figures 1A and 1B which depict a dendritic network and corresponding manhole loading hydrographs respectively.

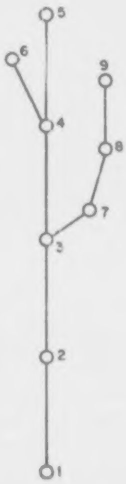


FIGURE 1A:
DENDRITIC
NETWORK

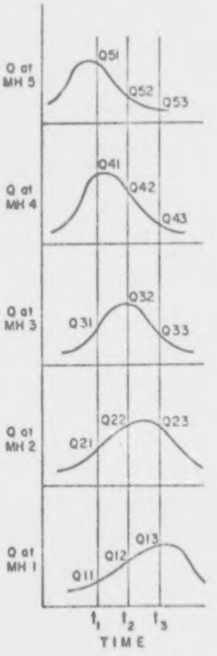


FIGURE 1B:
LOADING
HYDROGRAPHS

Water profiles by backwater means are determined at various time intervals t_1, t_2, t_3 and so on with t=0 being the start of the storm. In this manner, the worst profile for any sewer reach may be determined.

For time interval t_2, for example, the loading at Manhole 1 is Q12 obtained from the surface hydrograph contributing to Manhole 1. Similarly Q22 is obtained. At Manhole 3, the hydrograph includes the accumulation of the hydrographs at Manholes 3, 7, 8 and 9, taking into account the respective times of travel to Manhole 3. This methodology is continued to Manhole 5 at the upstream end of the system.

Within each manhole the following losses may be taken into account by SWAN:

1. Bend losses - varying with the upstream velocity head.
2. Change in velocity losses - due to the change in velocity heads and always positive.
3. Change in flow losses - due to an increase in flow caused by flow entering from a side strip.

If the sewer is surcharged because the flow is greater than the capacity, the piezometric head is defined by the energy gradient from the Hazen-Williams equation. If the surcharge is caused by downstream conditions and the conduit would normally carry the flow, the piezometric head is defined by the friction slope from the Manning equation.

The BACKWATER command is a very useful tool. Surcharged storm sewers can be shown to have larger capacities than that found by the Manning equation. A deep sewer can sustain a very large surcharge and perform with flows 100% higher than normal flow capacity. However, a constriction in a sewer can cause the capacity to be reduced for all upstream reaches. This may not be evident from analysis by other means.

Backwater techniques can be employed to analyze relief sewer capacity by simulating a surcharged system up to the piezometric head that equals the relieved sewer's overflow wiers. Overflow structures can be analyzed using this same approach.

These techniques should not be used when the surcharged piezometric head is in excess of three or four times the conduit diameter above the sewer crown. The assumptions are questionable under these conditions.

CONCLUSION

The use of SWAN on various projects since its inception in 1971 by Erdman, Anthony, Associates has shown it to be a valuable and accurate tool for the simulation of sewer flows. Its use, however, must be tempered with good engineering judgment, for it was not intended to circumvent the Engineer.

The implementation of SWAN can be a very useful and inexpensive method of keeping accurate records of a municipality's sewer networks. As the community grows, the data base can be expanded to include additions and improvements. Additions and improvements can be analyzed in the planning stages or checked in the design stage and thus reduce the chance of inadequate service. The municipal agency responsible for wastewater collection and disposal would have its network records and the procedures for analysis in one easily accessible source.

As the environmental movement picks up momentum and as more monies are made available for water pollution abatement, SWAN will be even more valuable to engineers and planners. Municipalities which do not have long-term statistical data available may employ SWAN to develop reasonably accurate models of critical events, and reduce the time from investigation to design.

It is the intent of the authors, depending of course on the availability of time and funds, to utilize the options of SWAN to compare the Rational Method with the Chicago Method and to determine their effects upon analysis and design. Several theoretical comparisons have been made, but to the knowledge of the authors, none have been made on actual complex and extensive sewer systems.

SWAN is a simple to use computer system which requires neither monstrous hardware nor tedious or complicated input form preparation. The output is neatly presented for ease of interpretation and the plotter features reduce the efforts of transferring computer output to hard copy. SWAN is upward compatible with respect to hardware within a FORTRAN environment. Lack of space prohibits a detailed description of SWAN and its related output. Those interested may feel free to contact the authors for further details.

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ON-LINE MODELS FOR COMPUTERIZED CONTROL
OF COMBINED SEWER SYSTEMS

J.W. Labadie and N.S. Grigg
Department of Civil Engineering
Colorado State University
Fort Collins, Colorado

P.D. Trotta
Department of Civil Engineering
University of Colorado
Denver, Colorado

Automatic computer control is a cost-effective approach to controlling polluting discharges from combined sewer systems. Perhaps the greatest challenge is development of programmable models and control logic that can find the best positioning of field control elements within the restrictions of the on-line, real-time environment. Control strategies can be developed off-line or on-line, and may be reactive or adaptive. It appears that simple reactive control, or rule curves, can adequately control total overflows, but may produce high overflow rates. Stochastic adaptive policies produce a smoother distribution of overflows, but are highly dependent on the accuracy of the storm inflow forecasting model. Autoregressive moving-average transfer function models are proposed as an efficient approach to forecasting. Initial indications are that total city-wide automatic control is feasible, both technically and economically.

Introduction

Increasing political and economic pressures are causing today's urban water manager to place a greater emphasis on cost-effectiveness of urban services and efficient spending of the public dollar. Accordingly, he has a great interest in searching for innovative solutions. It has been conclusively demonstrated that storm and combined sewer discharges are significant contributors to the total pollution reaching our receiving waters and the price tag to clean up these discharges has been estimated to be in the $200 billion range. Since neither this country as a whole nor individual cities can afford expenditures of this magnitude for the problem, better ways to manage existing systems and affordable new systems must be found.

Automatic computer control has been applied with success in industry for more than 15 years. It is only recently, however, that a few U.S. cities have implemented limited scale computer systems for controlling combined sewer overflows from portions of their urban complexes, with a number of other cities in various stages of planning for such systems.

It makes sense to consider automatic control of storage and flow in a combined sewer system by digital computer, especially in light of the tremendous advances made in recent years in industrial computer control. The availability of attractive computer hardware, however, does not by itself guarantee success in automating a system. The cost of such hardware may be the least of the costs involved.

The normal computer control project should proceed cautiously through phases, beginning with the simple to the more complex. The four basic levels of computer control can be listed as follows:

1. Data logging and processing
2. Conventional remote supervisory control
3. Automation of parts of systems and computer assisted control
4. Closed loop automatic computer control.

Once a commitment to the eventual implementation of automatic control is made, the greatest challenge is the development of programmable models and control logic that can ensure the most effective utilization of storage and treatment in the system. It is the control strategy development problem that is addressed herein.

Control Objectives

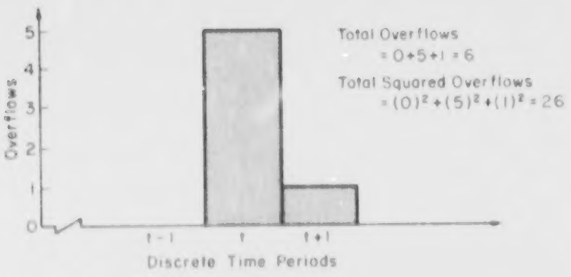
Application of automatic control to combined sewer systems requires that strategies be developed and implemented for remotely controlling adjustable valves, orifices, gates, and pumps within the system, during a real-time storm event, in such a way that certain control objectives are met as closely as possible, such as:

1. minimize the total volume of overflows reaching receiving waters during a storm event.
2. minimize the maximum rate of overflow discharge.
3. minimize the total mass of pollutants.
4. minimize the maximum rate of pollutant discharge.
5. minimize the detrimental impact of untreated overflows on the receiving water.
6. maximize the effective utilization of treatment plant, interceptor sewer, trunk sewer, and storage capacities.
7. minimize localized flooding from surcharged sewers.

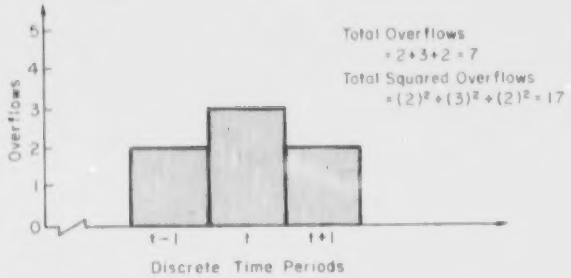
Objective 5, though highly desirable, is dependent on the availability of accurate models for predicting wastewater quality and its impacts on receiving waters. Such models may not be available, since water quality prediction is much more difficult than quantity modeling and prediction. Objectives 3 and 4 are also dependent upon wastewater quality prediction models. The City of Cleveland[2] has reported using Objective 3 for their control system. Utilization of Objective 4 might be an indirect means of satisfying 5, since it appears that the pollutant loading rate from discharges is more critical for receiving waters than the total mass of pollutants.

In the absence of adequate quality prediction models, one must settle for Objectives 1 or 2, used in conjunction with Objective 7. This latter objective is usually given a higher priority, due to the high nuisance level and sanitation problems associated with localized flooding and the fact that it *hits people where they live*. Sewer discharges leading to overflows, on the other hand, tend to pass *out of sight, out of mind*. It is obvious that any computer control system must be designed to control the system with regard to a proper tradeoff between overflow minimization objectives and localized flooding minimization objectives. Satisfaction of these objectives will indirectly satisfy Objective 6.

Figure 1 presents a simple example as a means of comparing Objectives 1 and 2. Suppose that application



a) Results of Objective 1



b) Results of Objective 2

Figure 1. Comparison of Objectives 1 and 2

of Objective 1 for optimal control of stormwater results in the overflow distribution shown in Figure 1(a), for some hypothetical real-time storm event. For Objective 2, an indirect means of minimizing the maximum overflow rate, or the total overflows during any discrete time period, is to minimize the sum of the *squared* overflows. This might result in an overflow distribution as shown in Figure 1(b), for the same storm event. Even though total overflows resulting from Objective 2 may be greater than those from Objective 1, the pollution shock on receiving waters may be less in the former case, where the maximum overflow rate is less.

Notice that in the case of Objective 2 (Figure 1(b)) overflows are taken during period t-1, even though there might be available storage capacity to store these flows. This is allowed in the interest of *smoothing out* the distribution of overflows so that impacts on the receiving waters are lessened.

Furthermore, multiplying overflows (or squared overflows) at particular points in time and space by *weighting factors* is an indirect way of considering pollution impacts. For example, bypass points with a history of overflows with higher pollutant concentrations could be assigned a higher weight than those for other bypass points. In this way, overflows are more heavily penalized at this location and therefore given a greater priority for control. Likewise, due to initial *flushing* effects, overflows occurring early in the storm event could be weighted more heavily than those occurring later. In addition, tidal or river level fluctuations might necessitate the adjustment of weighting factors. The utilization of weighting factors is a way of expressing subjective information in a quantitative manner, in the absence of accurate quality prediction models. It essentially is a means of setting up a priority scheme for allowing overflows when there is no choice but to allow them.

Objective 2, in a real-time context, could be indirectly expressed as:

$$\text{minimize} \quad \sum_{i=1}^{N} \sum_{t=m}^{M} \left\{ \omega_{it} \left[O^i(t) \right]^2 - cQ^i(t) \right\} \qquad (1)$$

where $O^i(t)$ are the total predicted overflows, as a result of some control policy, at bypass point i, during a discrete interval t ; ω_{it} are the weighting factors on overflow; N is the total number of bypass points; m is the current real-time interval since the storm began at $t=1$; M is some future time interval to which storm inflows are forecasted ($m \leq M$); $Q^i(t)$ are the predicted throughflows to treatment and c is a positive coefficient which *credits* throughflows and discourages unnecessary storage.

Control Constraints

Having specified the control system objectives, which must in some way be placed in quantitative terms, it is then necessary to specify the constraints under which the control system is to operate. These can be listed as follows:

1. The interceptor, trunk sewers, and detention storage devices have a limited capacity which, if exceeded, will result in localized flooding and untreated overflows.
2. The treatment plant(s) has (have) a maximum capacity for treating wet weather flow.
3. The transfer of rainfall to runoff to sewer flow operates under certain dynamic physical laws that can be approximated by mathematical models. In effect, these laws act as constraints on the control system.
4. The remote data acquisition system will have a limited capacity for retrieving and transferring information, both in time and space.
5. The hardware and software associated with the computer control system will have a limited capability.
6. The computer control system will have a restricted amount of *time* to render decisions in real-time and properly respond to a rapidly progressing storm event.
7. The system must operate under constraints of possible human error and equipment malfunction and breakdown.

The goal of the computer control system, then, is to meet the specified objectives as closely as possible, while operating under the above constraints. The design of the computer control system is therefore based on analysis of tradeoffs between cost of the system and its effectiveness in meeting the objectives under these constraints.

Off-Line vs. On-Line Control Development

The question that now arises is: how should computer control logic be developed in order to meet the above control objectives, subject to the constraints? There are two basic approaches to control logic development: off-line and on-line. By off-line development, we mean that the control policies are synthesized independently of the real-time control situation. That is, instead of programming the necessary mathematical models onto the real-time computing machinery, they are programmed onto batch-mode computing systems not interfaced with the actual control system. Many optimizations are then performed for an assumed range of probable storm events that could occur, based on historical or synthetically generated events. The resulting optimal strategies are then stored as rule curves in the on-line computer system for real-time control.

The *advantage* of off-line optimization is that sophisticated models of the sewer system and accurate analysis techniques can be used in an off-line manner, whereas it would be difficult to use them in an on-line computing system with limited hardware and time for making control decisions. The major *disadvantage* of off-line optimization is that its effectiveness is based on how well the range of predetermined storm events corresponds to what actually can occur in real-time. Obviously, there is an infinite number of possible events that can take place.

On-line development implies that the control optimization is actually carried out in real-time on the on-line computing system as a storm is passing over the urban area. The obvious advantage is that optimal controls can be developed that uniquely respond to the event at hand, as well as the current state of the sewer system in terms of flows and storage levels. The disadvantage is that simplified models and analysis techniques may be required because of hardware and software limitations of the on-line computing system (which might be a minicomputer, for example) and the limited time available to render control decisions.

Reactive vs. Adaptive Control Policies

Control policies resulting from off-line development tend to be *reactive* in nature. Other terms would be *local*, *set point*, or *myopic* control. That is, these kinds of control policies are *less* dependent on anticipation or forecasting of storm inflows. They simply react to the current flow situation. Some forecasting may be necessary if there are several rule curves programmed onto the computing system, and it is desired to select the best one for the current event, as well as modify it so some extent as the storm progresses.

On-line optimization implies a *greater* dependence on storm forecasting, as well as more extensive forecasting. The extreme would be an attempt to forecast future storm inflow rates over short time increments. Control policies based on on-line optimization might be termed *adaptive*. Though it is possible to have on-line optimization which is reactive (Brandstetter, et.al.[2]) and off-line control development which results in adaptive policies,[8] there is generally less emphasis on comprehensive forecasting in off-line development. It may be limited to forecasting only total depth and duration of the storm.

Adaptive control is based on the sequential and systematic updating of storm inflow forecasts as new information on the ensuing storm is gathered from an automated data acquisition system. Control policies can then be appropriately modified, based on the updated forecasts. In effect, then, a forecasting model is designed to be a *learning model* that can efficiently incorporate new information into its structure as it becomes available, so that succeeding forecasts ideally become better as real-time information on the storm event in progress is obtained.

The ultimate goal is what might be termed *stochastic adaptive control*. That is, instead of totally basing the evaluation of control policies on a forecasted storm event, it is recognized that there is considerable *uncertainty* (although a more appropriate term is *risk*) associated with that forecast, and this uncertainty tends to increase as we attempt to forecast further into the future. This approach is more realistic since if an *optimal* control policy is based on the certain occurrence of a sequence of future inflows, and it turns out that the actual inflows deviated considerably from the forecast, then the optimality of the control is in question. It would be better if a *band of uncertainty* (Figure 2) was associated with the forecast and a *stochastic* control policy development carried out which considered certain assumed probabilities of deviation from the most likely or expected levels of the forecast.

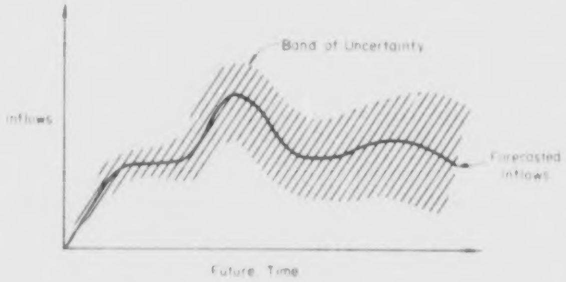


Figure 2. Inflow Forecasting Under Uncertainty (or Risk)

Under stochastic adaptive control in real-time, Equation 1 might be written as:

$$\text{minimize } E\left[\sum_{i=1}^{N} \sum_{t=m}^{M} \left\{\omega_{it}\left[O^i(t)\right]^2 - cQ^i(t)\right\}\right] \qquad (2)$$

where E denotes *expected value*.

On-Line Modeling Requirements

Rainfall-Runoff and Routing Models

Off-line control development can be based on either the simplest and most intuitive of analyses, or sophisticated studies involving mathematical models of system response. Given a set of historical or synthetic storm events, these rainfall data are passed through a *rainfall-runoff model* which predicts direct inflows to the sewer transport system. A *sewer routing model* is then required for predicting overflows.

Rainfall-runoff models range in sophistication from simple unit hydrographs to kinematic wave approaches (as in SWMM). Likewise, sewer routing models range from simple time-lag approaches to solution of the full unsteady flow equations (as in the San Francisco Stormwater Model (SFSM)[9]).

Again, off-line control development offers greater latitude in the degree of model sophistication, but results in more reactive type control. On-line control development, on the other hand, requires more simplified models, but can more uniquely respond to a current event in an adaptive mode.

The major limitation for on-line control is in the area of sewer transport routing. It is not yet feasible to solve the St. Venant equations on-line in real-time. Seattle[8] has found that the kinematic wave model developed for SWMM, modified to include backwater effects using simple continuity relationships, performed satisfactorily in real-time.

Forecasting Model

In addition to rainfall-runoff and sewer routing models, some kind of forecasting model is required for on-line control development. The more advanced models currently available attempt to describe the activity of storm *rain cells*, which can be defined as local areas of convective circulation resulting in more intensive rain. Rain cells in turn operate within larger areas of less intense rain called *bands*. A large collection of investigators have contributed to an understanding of the life cycle of cells within bands. An extensive bibliography on this subject can be found in Trotta[10]. The overall result of this rain cell research is that there appear to be definable statistical properties associated with rain cell activity. Since these models were primarily developed for simulation studies, there is some question as to their adaptability to real-time forecasting. The models tend to be large and time-consuming.

As an alternative to these comprehensive simulation models, certain techniques originating from electrical engineering may be applicable to rainfall forecasting. The two most important general forecasting approaches are (i) the extended Kalman filter, and (ii) the so-called autoregressive moving-average transfer function models. Graupe[4] has concluded that the latter models are preferable in terms of computational speed and simplicity, especially when certain aspects of the persistence or degree of autocorrelation of the inputs are not well understood, as is the case with stormwater forecasting.

Figure 3 gives a simple illustration of this approach. The regression relations are of the form (with the moving average terms deleted):

$$R^i(t+1) = a_0 R^i(t) + a_1 R^i(t-1) + \dots + a_p R^i(t-p) + \sum_{j \in J(i)} \Big[b_{0j} R^j(t) + b_{1j} R^j(t-1) + \dots + b_{sj} R^j(t-s) \Big] \qquad (3)$$

where t is the current real-time interval; $R^i(t+1)$ is the forecasted inflow; $J(i)$ is the set of all pertinent locations j adjacent to i ; $\underline{a}$ and $\underline{b}$ are parameters determined from historical data and the current storm event. These parameters can be easily updated in real-time, as shown by Trotta[10]. Though stationarity is assumed for the above model, nonstationarity can be considered by using a *differencing* operator. Equation 3 can be used sequentially to generate forecasts for any lead time.

In some cases it may be advantageous to forecast direct storm runoff rather than rainfall input. This is because the rainfall-runoff process tends to perform a smoothing and integrating action on rainfall input. These integrated data might be more conducive to analysis for forecasting purposes than rainfall data.

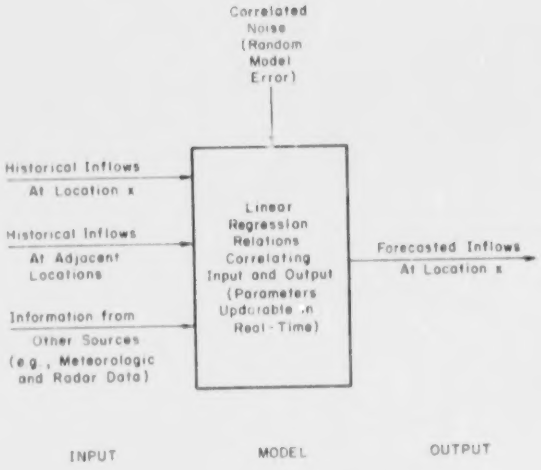

Correlated Noise (Random Model Error)
Historical Inflows
At Location x
Historical Inflows
At Adjacent Locations
Information from
Other Sources (e.g., Meteorologic and Radar Data)
Linear Regression Relations Correlating Input and Output (Parameters Updatable in Real-Time)
Forecasted Inflows
At Location x
INPUT
MODEL
OUTPUT

Figure 3. Illustration of Autoregressive Moving-Average Transfer Function Model

Optimizing Model

A quantified control objective and mathematical specification of all pertinent constraints on system response (including specification of some kind of sewer routing model), in conjunction with a systematic optimization algorithm for finding the best or near-best controls, is called an *optimizing model*.

The on-line control environment places restrictions on the degree of sophistication of the optimization algorithm, which in turn restricts the level of the mathematical models used (particularly the sewer routing model). The most popular optimization algorithm is the simplex method of *linear programming*, which has been applied by Bradford[1] to combined sewer control. Obviously, the use of linear programming constrains all sewer routing to be linear or piecewise linear. Nonlinear routing can be used with *dynamic programming*, but other computational difficulties arise.[7] Application of the *maximum principle* and *regulator theory*[3] is also a possibility, but routing also is a problem here.

Introducing stochastics further complicates the optimizing model. In addition, the city-wide control problem is large-scale and unwieldy, with many control variables. Labadie, et.al.[6] have proposed a hierarchical or multilevel optimization approach which can effectively deal with the large-scale problem.

Development of efficient, yet sufficiently accurate optimizing models for on-line use, remains a challenging area for future research.

Research Results and Conclusions

Intensive research on automatic control of combined sewer systems has been carried out at Colorado State University for the past five years. Work has primarily concentrated on the San Francisco Master Plan for Wastewater Management as a case study.

The most recent research results are described in Trotta[10]. The hierarchical approach to the control optimization is applied to the San Francisco system, where the urban area is divided into a number of subbasins which are essentially independent except for their contributions of storm runoff to a common interceptor and treatment facility. The controls for each subbasin are derived separately by the use of a stochastic dynamic programming formulation. Each subbasin problem, however, is constrained by an upper limit on its releases to the interceptor, which is determined by a master control problem. This master control problem, which ties together the separate subbasin problems, decides how interceptor and treatment capacity should be allocated to the subbasins. It uses a modified cyclic coordinate search algorithm. The inflows are forecasted using an autoregressive transfer function model which can be updated in real-time to respond to new information on the storm event.

The control algorithm was tested for selected design storms which were based upon the historic record. The tests were conducted on a batch-mode computer, but a hierarchy of minicomputers appears to be a more efficient approach to effecting the multilevel optimizations in real-time.

The results of this work indicate that the large-scale algorithm can converge within the time frame anticipated for real-time control. Controls based upon the stochastic models were superior to those based upon forecasts which were assumed deterministic. The adaptive aspects of the model appear to be justified by the superior distribution of the overflows which resulted when overflows were unavoidable. That is, the maximum rate of overflow was lowest for this model. This result is notable in that the forecasting model was deliberately designed to be relatively inaccurate. Total overflows were, however, minimized to a higher degree by a reactive model which was also tested, though the maximum overflow rate was higher. The overall conclusion appears to be that even though the adaptive model with risk is highly dependent on the accuracy of the forecasting model, at least some stormflow anticipation will reduce maximum overflow rates. Thus, reactive policies better meet Objective 1, as long as weighting factors are not used, and stochastic adaptive policies are superior for Objective 2.

As illustrated in Figure 4, if a storm event is definitely considered to be non-overflow producing, then simple rule curves or reactive policies are adequate. If a storm is definitely overflow producing, rule curves tend to produce higher rates of overflow than stochastic adaptive policies. There is, of course, a gray area in between, the size of which depends on the accuracy of the forecasting model. The safest procedure in these gray areas is to use reactive policies, since if the forecasting model is relatively inaccurate, unnecessary overflows may be taken.

Initial cost estimates presented in Grigg, et.al.[5] show that computer hardware would cost around $200,000 for implementing the proposed city-wide hierarchical control strategy for San Francisco. Software, development costs would be about the same, for a total of $400,000. This is a relatively insignificant amount, in comparison with total project costs that could approach $1 billion.

Acknowledgments

The financial support of the National Science Foundation (Research Applied to National Needs) and the Office of Water Research and Technology, Department of Interior, are gratefully acknowledged. Much of the data which made the research possible were furnished by the Department of Public Works, City and County of San Francisco. In addition, the technical advice and assistance provided by Mr. Murray B. McPherson, Director, ASCE Urban Water Resources Research Program, was instrumental in stimulating the research.

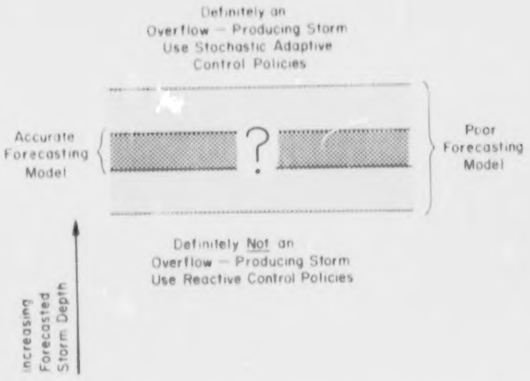


Figure 4. Effect of Forecasting Model Accuracy on Control Policy Selection

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MATHEMATICAL MODELS FOR CALCULATING PERFORMANCE AND COST OF WASTEWATER TREATMENT SYSTEMS

Richard G. Eilers
Systems and Economic Analysis Section
Wastewater Research Division
Municipal Environmental Research Laboratory
U.S. Environmental Protection Agency
Cincinnati, Ohio

ABSTRACT

The Systems and Economic Analysis Section of the Wastewater Research Division of EPA in Cincinnati, Ohio is concerned with finding quantitative expressions for calculating the performance and cost of wastewater treatment processes as a function of the nature of the wastewater to be treated and the design variables associated with the individual unit processes. These models are intended primarily to characterize the treatment of municipal sewage. Since the procedure for solving all of the quantitative equations is usually too laborious or complex to be accomplished by hand calculation, various FORTRAN computer programs have been developed to perform the task.

BACKGROUND

Mathematical models for wastewater treatment processes are required to express the performance of the processes over the full range of operational modes and design criteria. These models can be steady state, quasi-steady state, or time-dependent. By quasi-steady state it is meant that a steady state model is used to simulate a process that is, in reality, not necessarily steady state. Most sewage treatment systems are not steady state. The time-dependent or dynamic models are of interest when the quality of the effluent stream from a process is important as a function of time, or when the effectiveness of various kinds of control schemes on a process is being studied.

For a model to be fully effective for design and planning purposes, it must be based on valid scientific principles, flexible enough to simulate experimental data from a full-scale process (not merely pilot-scale data), and represent the performance and cost of the process with adequate precision.

The collection of valid, complete experimental data followed by adjustment of the model parameters to make the computed results agree with experimental results within an acceptable tolerance is also an important phase of model development.

Packaging mathematical models as computer programs not only provides ease and accuracy of calculation, but also has the additional advantage of convenience of distribution to interested individuals, such as consulting engineers and urban planners, in a readily usable form.

MODELS DEVELOPED

Over the past eight years, a number of computer models have been developed in-house by the Systems and Economic Analysis Section and through contracting activity with outside sources. Each program deals in some way with the cost and/or performance of wastewater treatment systems. All of the computer programs were written in FORTRAN and designed to run on a 16K IBM 1130 machine, and supporting documentation has been prepared for each. Table 1 gives a listing of the models which were produced in-house, and Table 2 shows the models which resulted from extramural sources. A brief description of the most significant of these computer programs will follow.

Table 1. Computer programs produced by the Systems and Economic Analysis Section.

1. Preliminary Design and Simulation of Conventional Wastewater Renovation Using the Digital Computer (1968).
2. Executive Digital Computer Program for Preliminary Design of Wastewater Treatment Systems (1968).
3. A Mathematical Model for a Trickling Filter (1969).
4. Preliminary Design of Surface Filtration Units-Microscreening (1969).
5. A Generalized Computer Model for Steady State Performance of the Activated Sludge Process (1969).
6. Fill and Draw Activated Sludge Model (1969).
7. Mathematical Simulation of Ammonia Stripping Towers for Wastewater Treatment (1970).
8. Mathematical Simulation of Waste Stabilization Ponds (1970).
9. Simulation of the Time-Dependent Performance of the Activated Sludge Process Using the Digital Computer (1970).
10. Economics of Consolidating Sewage Treatment Plants by Means of Interceptor Sewers and Force Mains (1971).
11. Per Capita Cost Estimating Program for Wastewater Treatment (1971).
12. Wastewater Treatment Plant Cost Estimating Program (1971).
13. Design of Concrete and Steel Storage Tanks for Wastewater Treatment (1971).
14. Water Supply Cost Estimating Program (1972).
15. Cost of Phosphorus Removal in Conventional Wastewater Treatment Plants by Means of Chemical Addition (1972).
16. A Mathematical Model for Aerobic Digestion (1973).
17. Design and Simulation of Equalization Basins (1973).
18. Mathematical Model for Post Aeration (1973).
19. Optimum Treatment Plant Cost Estimating Program (1974).
20. Waste Stabilization Ponds Cost Estimating Program (1974).

21. Granular Carbon Adsorption Cost Estimating Program (1974).
22. Control Schemes for the Activated Sludge Process (1974).
23. Cost Estimating Program for Disinfection by Ozonation (1974).
24. Nitrification/Denitrification Cost Estimating Program (1975).
25. Cost Estimating Program for Alternate Oxygen Supply Systems (1975).
26. Cost Estimating Program for Land Application Systems (1975).
27. Combustion Model for Energy Recovery from Sludge Incineration (1975).
28. Energy Consumption by Wastewater Treatment Plants (1975).
29. Stream Model for Calculating BOD and DO Profiles (1976).

Table 2. Computer programs produced as a result of contract activity.

1. Ammonia Stripping Mathematical Model for Wastewater Treatment (1968).
2. Mathematical Model for Wastewater Treatment by Ion Exchange (1969).
3. Mathematical Model of the Electrodialysis Process (1969).
4. Mathematical Model of Tertiary Treatment by Lime Addition (1969).
5. Mathematical Model of Sewage Fluidized Bed Incinerator Capabilities and Costs (1969).
6. Reverse Osmosis Renovation of Municipal Wastewater (1969).
7. Methodology for Economic Evaluation of Municipal Water Supply/Wastewater Disposal Including Considerations of Seawater Distillation and Wastewater Renovation (1970).
8. Mathematical Model of Recalcination of Lime Sludge with Fluidized Bed Reactors (1970).
9. Computerized Design and Cost Estimation for Multiple Hearth Incinerators (1971).
10. Cost program for Desalination Process (1971).

EXECUTIVE PROGRAM

The major product of all this effort has been the "Executive Digital Computer Program for Preliminary Design of Wastewater Treatment Systems." It was realized that a tool was needed which would allow the process designer to select a group of unit processes, arrange them into a desired configuration, and then calculate the performance and cost of the system as a whole. The Executive Program meets this need by simulating groups of conventional and advanced wastewater treatment unit processes arranged in any logical manner. Each unit process is handled as a separate subroutine which makes it possible to add additional process models to the program as they are developed. There are presently 24 process subroutines in the program, and these are listed in Table 3. Additional subroutines are planned to be included in the future, and a tentative list is shown in Table 4.

The first step in using the Executive Program is to draw the desired system diagram showing the unit processes to be used and the connecting and recycle streams. All streams and processes are then numbered by the program user. Figure 1 depicts a typical, conventional activated sludge treatment system with incineration for sludge disposal. Volume and characteristics of the influent stream to the system and design variables for each process used must be supplied as program input. By an iterative technique, each process subroutine is called in the proper sequence and all stream values are recomputed until the mass balances within the treatment system are satisfied. Performance, cost, and energy requirements for each unit process and the system as a whole are included in the final printout.

Table 3. Unit process models contained in the Executive Program.

1. Preliminary Treatment
2. Primary Sedimentation
3. Activated Sludge-Final Settler
4. Stream Mixer
5. Stream Splitter
6. Single Stage Anaerobic Digestion
7. Vacuum Filtration
8. Gravity Thickening
9. Elutriation
10. Sand Drying Beds
11. Trickling Filter-Final Settler
12. Chlorination-Dechlorination
13. Flotation Thickening
14. Multiple Hearth Incineration
15. Raw Wastewater Pumping
16. Sludge Holding Tanks
17. Centrifugation
18. Aerobic Digestion
19. Post Aeration
20. Equalization
21. Second Stage Anaerobic Digestion
22. Land Disposal of Liquid Sludge
23. Lime Addition to Sludge
24. Rotating Biological Contactor - Final Settler

Table 4. Unit process models to be added to the Executive Program

1. Ammonia Stripping of Secondary Effluent
2. Granular Carbon Adsorption
3. Ion Exchange
4. Electrodialysis
5. Reverse Osmosis
6. Bar Screening
7. Comminution
8. Grit Removal
9. Flow Measurement
10. Waste Stabilization Ponds
11. Microscreening
12. Rough Filtration
13. Multi-Media Filtration
14. Ozonation
15. Nitrification
16. Denitrification

Detailed cost data applicable for preliminary design estimates are generated by the Executive Program. Construction cost (in dollars), amortization cost, operation and maintenance cost, and total treatment cost (all in cents per 1,000 gallons of wastewater treated) are calculated individually for every unit process, and a sum total of each cost is given for the entire system. Capital cost is also computed by adding onto construction expenses the costs of yardwork, land, engineering, administration, and interest during construction. All of the cost information can be updated or backdated with respect to time by means of cost indices that are supplied as input to the program.

The Executive Program cannot be used for extremely detailed design purposes. However, it can be a valuable preliminary design tool for the consulting engineer or planner. The performance of existing or proposed wastewater treatment plants can be simulated along with providing cost estimates for building and operating these plants. It is also possible to optimize a particular treatment system by varying design parameters and noting the effect on performance and cost. Cost-effectiveness studies can be made by comparing alternate treatment systems. Initial studies along these lines are becoming of increasing importance because of the soaring costs of plant construction that are now being experienced.

A recent application of the Executive Program was an investigation of the potential economic advantages associated with 261 different methods for treating and disposing of sewage sludge. Sludge production and the costs of constructing and operating the various systems were computed. Each system was either primary or activated sludge treatment followed by some combination of the following 12 sludge handling processes--lime stabilization, gravity thickening, air flotation thickening, single-stage anaerobic digestion, two-stage anaerobic digestion, aerobic digestion, elutriation, vacuum filtration, centrifugation, sludge drying beds, multiple hearth incineration, and land disposal of liquid sludge. The outcome of the study showed that the cost (in January 1974 dollars per ton of dry solids processed) for treating and disposing of sewage sludge ranges from about $30 per ton for anaerobic digestion followed by dewatering on sand drying beds to over $100 per ton when the sludge is dewatered by vacuum filtration or centrifugation and then incinerated. Treatment and disposal of sludges produced in municipal wastewater treatment plants were shown to account for as much as 60% or as little as 20% of the total cost of treatment. Therefore, careful consideration should be given to selecting the sludge handling method which meets the site-specific constraints at a minimum cost. The Executive Program, which is capable of examining the cost and performance of a wide variety of alternative sludge handling schemes, can be used as a management tool to narrow the range of options when design conditions are known.

The Executive Program has been around for several years now, beginning with its original development in 1968. The model has been expanded, modified, and corrected many times since then, and it will continue to change in the future. The goal will remain the same: to provide the best possible characterization of the cost and performance of municipal wastewater treatment systems.

MODELS FOR THE ACTIVATED SLUDGE PROCESS

Considerable effort has been expended in developing more accurate models for the activated sludge-final settling process. Previous models that were produced by various researchers covered a wide range of forms corresponding to differing sets of assumptions about the hydraulic and biological relationships believed to be significant in the process. Because of the problems of measurement and the difficulty of fitting data to complex models, simplified models were often used which either omit or make some plausible assumption concerning the role of various factors in the process.

In all, four different digital computer models for the activated sludge process have been developed. The first, CSSAS (Continuous Steady State Activated Sludge), is a steady state model which is flexible enough to simulate the performance of any configuration proposed (complete mix, plug flow, multiple aeration tanks, step aeration, step return flow, contact stabilization, extended aeration, etc). Two classes of microorganisms are considered: heterotrophs which use 5-day BOD as substrate and Nitrosomonas which use ammonia nitrogen as substrate to produce new cells. The model allows the maximum rate constant for synthesis to vary with process loading. The second program, FADAS (Fill and Draw Activated Sludge), attempts to simulate the biological activity in a fill and draw bench experiment where activated sludge is mixed with substrate in any proportion. The third program, TDAS (Time-Dependent Activated Sludge), simulates the dynamic behavior of the biological aspects of the activated sludge process. The model numerically integrates the mass balance and biological rate equations which are assumed to represent the process. Three classes of microorganisms are considered: heterotrophs, Nitrosomonas, and Nitrobacter. This model can also be used to investigate the potential advantages associated with the following control schemes: dissolved oxygen control, sludge wasting control, and sludge inventory control. The fourth program, CMAS (Completely Mixed Activated Sludge), is used to simulate the performance of conventional and modified activated sludge, separate nitrification, or separate denitrification. With an adjustment of the process parameters, it can also be used to characterize the pure oxygen activated sludge system.

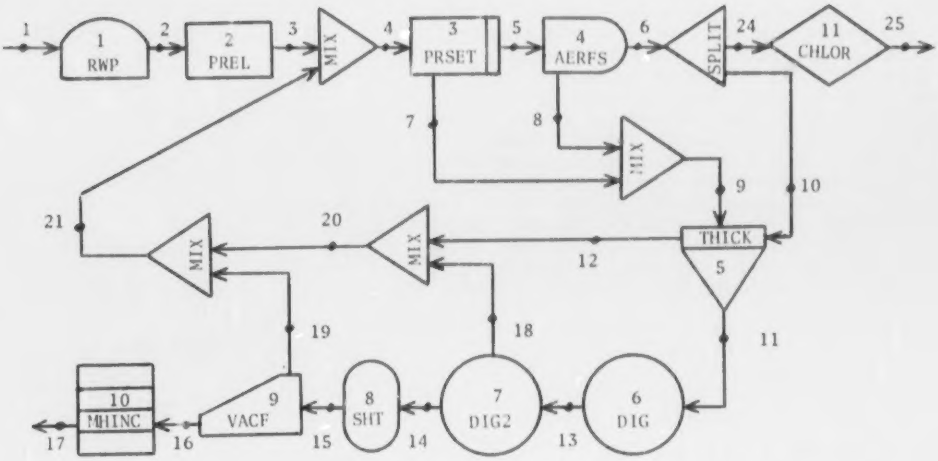
SPECIALIZED COST ESTIMATING PROGRAMS

When making preliminary cost estimates for building and operating certain wastewater treatment systems, it is often necessary to have more detailed cost data. For this reason, special economic models were developed for several particular applications.

A waste stabilization pond cost estimating program computes the costs of stabilization ponds and aerated lagoons along with influent pumping, surface mechanical aerators, embankment protection, and chlorination facilities. The granular carbon adsorption cost estimating program calculates the costs of influent pumping, carbon contactors, regeneration facilities, and initial carbon required. The nitrification/denitrification cost estimating program predicts the costs of dispersed floc systems for the removal of nitrogen from wastewater. A cost estimating program for wastewater treatment by direct land application computes the costs of preapplication treatment, transmission, storage, field preparation, distribution, renovated water recovery, and monitoring facilities. All of these economic models factor in the costs of yarkwork, contingencies, engineering, land, administration, and interest during construction.

CONCLUSION

The primary goal of this modeling effort is to improve the rule-of-thumb or hand calculation method of process design which is still commonly used today. The principal deterrents to better process design are usually the manual effort required in computing the cost and performance of alternative designs and the labor required to accumulate and correlate the large amount of experimental process design performance data which is often available. The mathematical computer model can minimize the computational work required for examining alternative designs, and, if the model has been correctly developed, it will reflect the best experimental and scientific information obtainable. Thus, the process designer has within his grasp the tools for quantitatively selecting the most cost-effective system of processes to achieve any desired wastewater treatment goal. The Systems and Economic Analysis Section within EPA is very much interested in promoting the use of computerized design techniques in order to achieve better treatment at a minimum cost.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8 SHT
7 DIG2
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RWP - raw wastewater pumping
PREL - preliminary treatment
MIX - stream mixer
PRSET - primary sedimentation
AERFS - activated sludge/final settler
SPLIT - stream splitter
CHLOR - chlorination/dechlorination
THICK - gravity thickening
DIG - single stage anaerobic digestion
DIG2 - second stage anaerobic digestion
SHT - sludge holding tanks
VACF - vacuum filtration
MHINC - multiple hearth incineration

Figure 1. System diagram for a conventional activated sludge treatment plant.

THE ECOLOGICAL MODEL AS APPLIED TO LAKE WASHINGTON

Carl W. Chen
Tetra Tech, Inc.
Lafayette, California

Donald J. Smith
Tetra Tech, Inc.
Lafayette, California

INTRODUCTION

A lake is a giant reactor where many physical, chemical and biological processes take place. Heating and cooling at the water surface due to solar insolation, conductance, back radiation and evaporation generate the thermal stratification and seasonal overturn phenomenon. Thermal stratification separates the lake water into layers with different physical, chemical, and biological characteristics. It influences where the tributary inflows are deposited and where outflows are withdrawn.

Tributary inflows bring in plant nutrients (carbon, nitrogen and phosphorus) either in the dissolved form or as particulate organic matter. Bacteria or fungi decompose organic matter to liberate nutrients and consume oxygen in the process. With the help of solar energy, phytoplankton reuse the nutrients to synthesize new organic materials and produce oxygen. Under stratified conditions, phytoplankton activity predominates in the epilimnion (above the thermocline) and bacterial activity predominates in the hypolimnion, creating an imbalance for oxygen resources. At the surface, the water may be saturated with oxygen, but the hypolimnion water may become anerobic, killing fish and other organisms residing near the bottom.

Biomass generated by bacteria and phytoplankton serve as food for zooplankton, benthic animal and fish. Carbon, nitrogen and phosphorus contained in the biomass are conserved in each succession of organisms. Upon death, they become organic materials to be worked at by bacteria.

This paper describes an ecological model that simulates the physical, chemical and biological processes of the complex lake ecosystem. The model represents the state of ecosystem by a set of water quality parameters including biomass of various organisms. The model calculates throughout the annual cycle the vertical profiles of temperature, dissolved oxygen, biochemical oxygen demand (BOD), pH, plant nutrients (CO_2, NH_3, NO_2, NO_3, PO_4), particulate organic matter, organic sediment, algae, zooplankton, benthic animals, and fishes.

The model provides a scientific tool for engineers to evaluate effectiveness of various management alternatives. It also serves for the multidisciplinary integration of bits and pieces of information that has been accumulated in various branches of sciences, i.e., meteorology, hydrology, hydrodynamics, limnology, ecology, chemistry, biology, and sanitary engineering.

Lake Washington data, collected by Dr. Edmondson of the University of Washington, were used for the model calibration and sensitivity analyses.

LAKE WASINGTON

Lake Washington has a surface area of 110 x 10^6 m^2 and a volume of 3.6 x 10^9 m^3. It has a maximum depth of 65 m.

Figure 1 shows the location of Lake Washington and its tributaries including waste water discharges and storm water overflows. As shown, the Sammamish River enters the lake in the north and the Cedar River in the south. Numerous small creeks empty into the lake for the local drainage. The outflow is regulated by the ship canal connecting the lake and Puget Sound. Table 1 summarizes the inflow and outflow hydrology of Lake Washington.

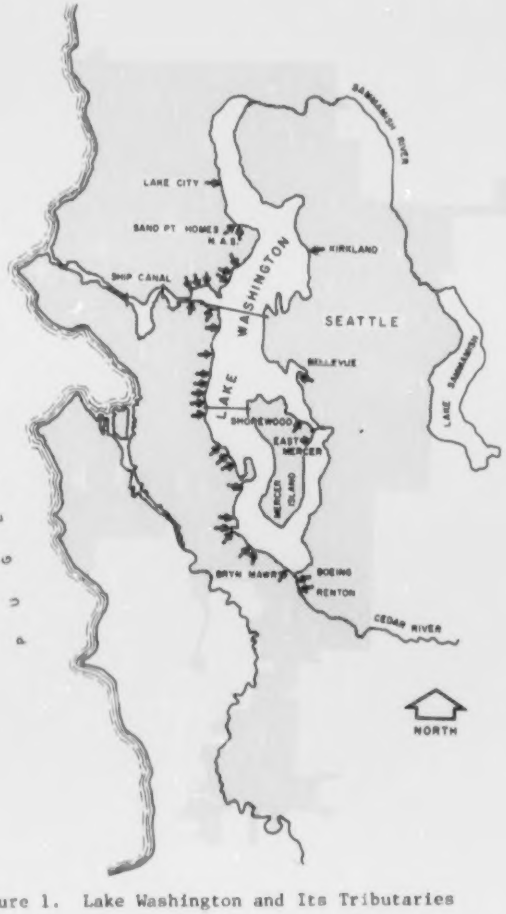


Figure 1. Lake Washington and Its Tributaries

Table 2 presents the mean monthly weather conditions for the years 1966 and 1967 as observed at the Tacoma Airport. The weather conditions are assumed the same as those experienced by the lake.

In 1941, the lake received one discharge of secondary effluent. By 1963, the sewage discharge reached about 0.53-0.75 CMS (cubic meter per second) or 12-17 MGD (million gallons per day), exclusive of combined storm water overflows. In 1963, sewage diversion began and by February, 1968 all sewage was exported.

Table 1. Inflow and OUtflow Hydrology

Month	Sammamish River	Cedar River	Local drainage	Lake City^b	Bellevue^b	Bryn Mawr^b	Septic tank	Outflow
January	20	33.6	8.5	0.6	0.13	0.11	0.011	62.0
February	22	35.0	10.0	0.5	0.13	0.10	0.011	62.0
March	18	23.0	7.0	0.45	0.11	0.08	0.011	60.0
April	14.6	25.2	5.6	0.4	0.11	0.08	0.011	45.0
May	9.1	24.0	3.4	0.35	0.10	0.08	0.011	35.0
June	6.0	30.0	2.3	0.32	0.09	0.08	0.011	30.0
July	4.5	10.0	1.5	0.30	0.07	0.07	0.011	27.0
August	3.5	10.0	1.3	0.30	0.09	0.08	0.011	25.0
September	3.5	8.5	1.5	0.3	0.09	0.10	0.011	23.0
October	5.0	15.0	2.0	0.3	0.10	0.10	0.011	25.0
November	10	25.0	4.5	0.35	0.11	0.10	0.011	30.0
December	18	35.5	7.0	0.55	0.1	0.11	0.011	50.0

[a] All flows are in cubic meters per second; multiplying 35.31 to cfs and 22.8 to mgd.

[b] The Lake City discharges include Sand Point Homes and Kirkland; the Bellevue discharges include Shorewood and East Mercer, and the Bryn Mawr discharges include Boeing and Renton.

Table 2. Weather Conditions at Tacoma Airport

Month	Atmospheric pressure mbar	Cloud cover %	Shortwave^a radiation kcal m^-2	Longwave^a radiation kcal m^-2	Dry bulb temp °C	Wet bulb temp °C	Wind speed m sec^-1
January	1015	92	0.009	0.065	4.8	2	3.6
February	1017	80	0.020	0.065	6.3	2	3.5
March	1016	77	0.034	0.065	7.5	2.6	3.5
April	1020	67	0.043	0.068	9.5	5.0	3.0
May	1018	60	0.052	0.070	11.0	6.6	3.0
June	1017	76	0.015	0.075	15.0	9.2	2.8
July	1016	60	0.065	0.080	18.0	11.4	2.5
August	1018	52	0.038	0.078	18.0	11.8	2.4
September	1018	61	0.042	0.075	15.0	12.2	2.3
October	1019	77	0.020	0.070	12.0	7.8	2.[illegible]
November	1015	86	0.011	0.068	8.5	5.2	2.8
December	1014	94	0.008	0.065	5.4	4.6	3.0

[a] Computed from longitude 47.36N, latitude 122.3W, sun angles, and cloud covers for 1966-67

The secondary effluent contained 4-12 mg/l of phosphorus, 8-20 mg/l of nitrogen, and 5-25 mg/l of BOD. In 1963, sewage contributed about 84% of the total phosphorus and 40% of the total nitrogen input to the lake. The total annual phosphorus and nitrogen inputs were estimated at 120,000 kg and 220,000 kg respectively.

According to Edmondson's data, the lake water is well mixed horizontally. A set of historical water quality data have been furnished by Edmondson for this study.

ECOLOGICAL MODEL

The concepts of the ecological model have been presented previously by Chen (1). A detailed description of modeling approaches, mathematical formulation and solution techniques can be found elsewhere (2).

Basically, the physical geometry of the lake is represented by stacked layers of water. Layers are added or deleted with the rise or fall of the water surface. The cross sectional area, volume, width and side slope of each layer are input items.

Water quality parameters are defined for each layer, and are expressed in the appropriate unit. The object of the model is to calculate the parameter values for each layer as a function of time.

To facilitate the computation, differential equations are developed to describe the changing rate of mass concentration or heat content as a function of such physical processes as 1) deposition of tributary inflow; 2) withdrawal of outflow; 3) advection between layers; 4) diffusion between layers; 5) sedimentation, if any, from the upper layer to the lower layer; 6) reaeration of the surface (CO_2 and O_2); and 7) solar insolation near the surface.

Deposition of tributaries and the concomitant advection are idealized by Figure 2 which shows the sinking of the inflow to an appropriate layer with approximately the same density.

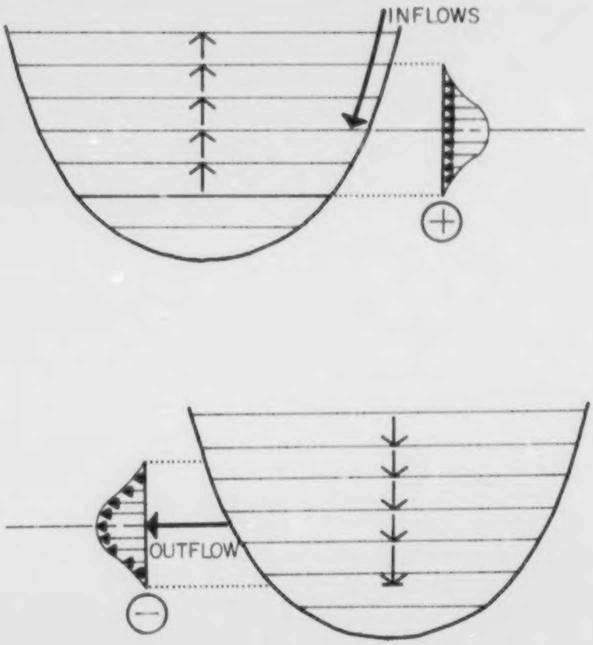


Figure 2. Inflows, Outflows, and Concomitant Advection

In addition, the mass concentration of quality constituents can be modified by the biological processes of 1) the oxidation of ammonia, nitrite, BOD, and detritus; 2) photosynthetic oxygenation, nutrient uptake and release of algae; and 3) the growth, mortality, and respiration of zooplankton, fish and benthic animals. The biological processes are usually represented by the product function of a temperature dependent coefficient and the mass concentration of the reacting constituents. For the biological parameters, the growth rate is expressed by a hyperbolic function of the substrate concentration.

Resulting differential equations are typically of the form

$$\frac{d(VC)}{dt} = f\left(Q, E\frac{dc}{dz}, S\right)$$

where: V = water volume
C = mass concentration or water temperature
t = time
Q = advective flows
$E\frac{dc}{dz}$ = diffusion between layers
S = various quality constituents, sources, sinks, and chemical, physical and biological reactions within each layer

There are as many equations as there are quality constituents and physical layers modeled. Numerical solutions are provided by the computer program which calculates C's from an initial time (t_o) to a short increment of time ($t_o = \Delta t$), in a recursive manner. Time step of computation can be as long as a day.

The output contains the vertical distribution of temperature, dissolved oxygen, BOD, alkalinity, pH, CO_2, NH_3, NO_3, PO_4, coliform, algae (2 groups), zooplankton, detritus, TDS, organic sediment and benthic animals. Fish productivity, evaporation loss, and formation are calculated for the surface on a per unit area basis.

SIMULATION RESULTS

The model was applied to simulate 1) the pre-diversion condition of sewage from Lake Washington; 2) the recovery of the lake after sewage diversion; 3) the sensitivity analyses.

Pre-diversion Case

Figure 3 shows the observed and computed temperature profiles throughout the annual cycle. The comparison is good considering that the mean weather conditions have been used as the model input.

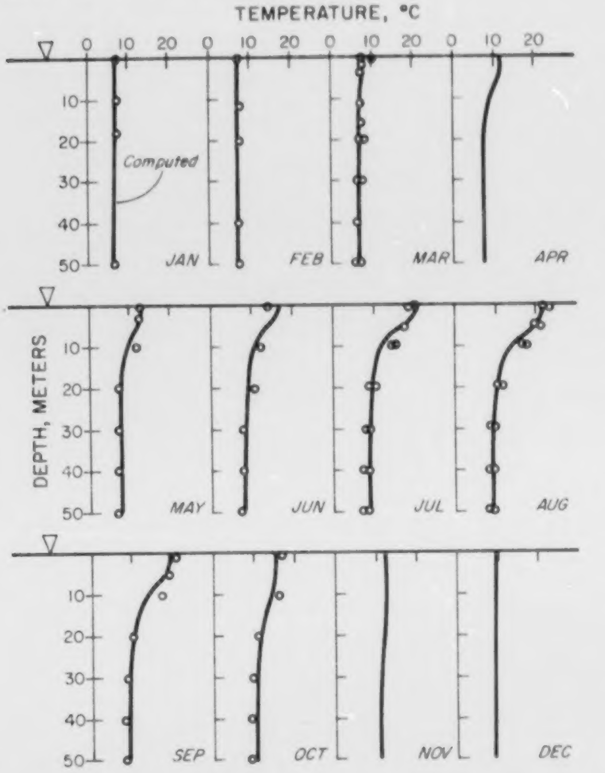


Figure 3. Calculated and Observed Temperature Profiles

Figure 4 plots the concentration profiles of dissolved phosphorus as observed in the field and computed by the model. Upon the onset of thermal stratification, the dissolved phosphorus at the surface is seen to be consumed by algae, creating a reversed concentration profile.

Other quality profiles that have been plotted to illustrate the reasonableness of the model include dissolved oxygen (DO), nitrate, and ammonia.

Lake Recovery

The model was set up to simulate the lake recovery after sewage diversion. It was run for a time period of three years. Sewage input was imposed during the first year and excluded for the last two years. All other boundary conditions remained the same.

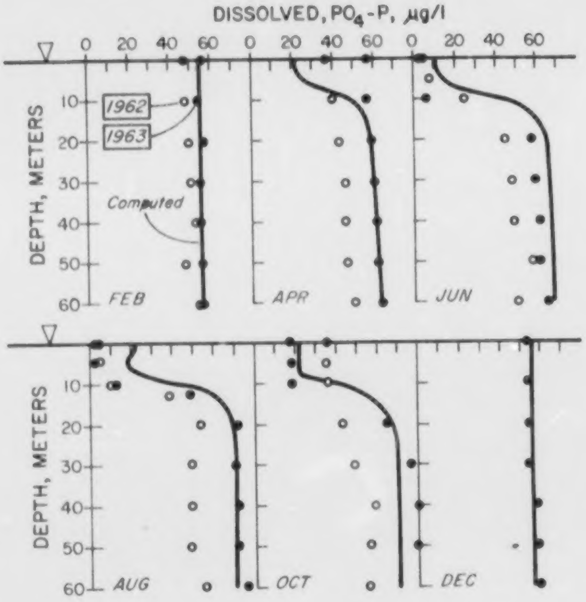


Figure 4. Calculated and Observed Concentation Profiles of Phosphorous

Figure 5 shows the model responses for P, N, DO, algae and pH at the surface and hypolimnion. Representative data observed during the pre-diversion years are plotted with the first year results and those observed during the post-diversion years are plotted with the third year results

The rapid recovery of the lake is predicted adequately by the model. The end of year phosphorus concentration is seen to reduce from 59 μg/l to 45 μg/l in one year and to 37 μg/l in two years after diversion. Nitrogen levels were reduced from 440 μg/l to 420 μg/l to 415 μg/l.

The minimum hypolimnion DO improves from 1.9 mg/l to 3.5 mg/l. The algal density is shown to reduce from 3.0 mg/l to 2.2 mg/l. The observed chlorophyl a level, converted to biomass by an approximate factor of 1:20, was shown to have a dramatic reduction in 1967 as predicted.

Sensitivity Analyses

During the early phase of model development, the half saturation constant of CO_2 was estimated at 0.6 mg/l carbon. The CO_2 exchange rate at the air-water interface was assumed to be 90% of the oxygen reaeration rate.

As a result, the model never predicted a pH higher than 8.4 during the summer. To maintain a pH of 9.2 in the summer as observed by Edmondson, the sensitivity analysis indicated that the CO_2 exchange rate should be 10% of the oxygen reaeration rate. The half saturation constant for CO_2 should be 0.025 mg/l carbon. The latter value has been confirmed by laboratory study (3).

To assess the relative importance of oxygen sinks in the hypolimnion, model simulations were performed with 1) the doubled decay rates of detritus and organic sediment; 2) algal respiration rate reduced to zero;

and 3) eliminating the waste input without modification of the initial conditions.

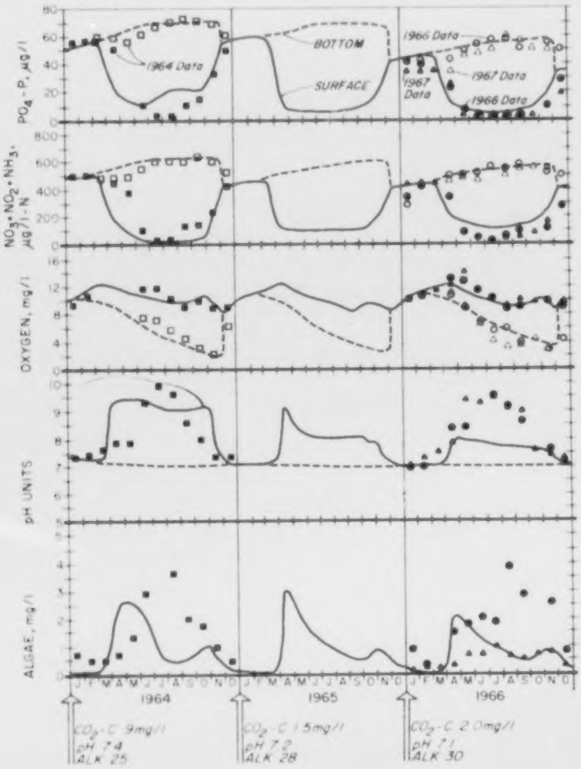


Figure 5. Recovery of Lake After Sewage Diversion

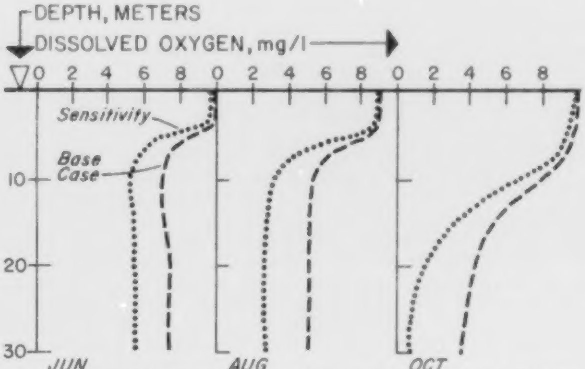
Model responses of DO profiles are presented in Figure 6. The most important sinks of hypolimnion DO are the respiration of algae and the decay of organic materials accumulated in the bottom.

The waste inputs appear to contribute very little to the direct oxygen consumption. They stimulate the growth of algae which settles and respires in the hypolimnion.

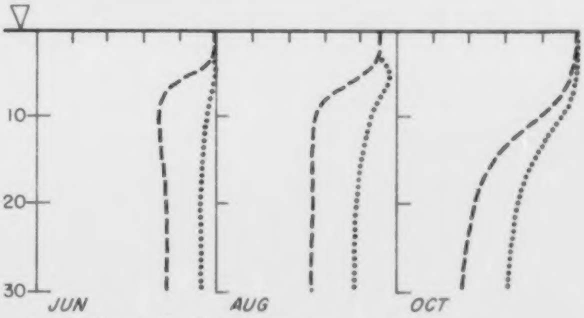
SUMMARY AND CONCLUSIONS

A general purpose water quality ecological model was developed and applied to Lake Washington. The model represents the Lake as stacked layers of hydraulic elements. Hydraulic routing, heat budget and mass balance computations are performed with a daily time step throughout the annual cycle. The output contains the vertical distribution of temperature, dissolved oxygen, BOD, alkalinity, pH, CO_2, NH_3, NO_3, PO_4, Coliform, algae (2 groups), zooplankton, detritus, TDS, organic sediment, and benthic animal. The evaporation loss, ice formation, surface algal productivity, and fish productivity for cold, warm and benthic fishes are also calculated.

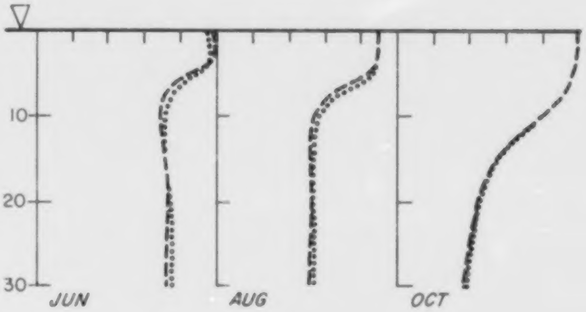
Application of the model to pre and post diversion cases of sewage from Lake Washington indicates the validity of the results as compared to Edmondson's data. Sensitivity analyses indicate that half saturation constant for CO_2 should be 0.025 mg/l. The sinks of hypolimnion oxygen are equally divided between the decay of organic materials accumulated near sediment and the respiration of settling algae. The model predicts the rapid recovery of the lake due to the flushing effects of tributary inflows.



a. Increased Decay Rates of NH_3, NO_2, BOD, Detritus



b. Reduced Algal Respiration



c. Reduced Waste Load Input

Figure 6. Model Responses to Sensitivity Analyses

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A LIMNOLOGICAL MODEL FOR EUTROPHIC LAKES AND IMPOUNDMENTS

Robert G. Baca
Water and Land Resources Department
Battelle-Northwest Laboratories
Richland, Washington

Ronald C. Arnett
Research Department
Atlantic Richfield Hanford Company
Richland, Washington

ABSTRACT

A general limnological model is formulated in terms of key environmental variables including dissolved oxygen, biochemical oxygen demand, temperature, phytoplankton, zooplankton and the principal nutrients. The major controlling factors such as light, temperature, nutrient loading rates, sediment interactions, and flow patterns are integrated into the model formulation to provide a detailed portrayal of the important limnetic processes. The model formulation is generalized to apply to well-mixed and stratified systems. The capabilities of the limnological model are demonstrated with applications to three lakes: Lake Washington near Seattle, Lake Mendota and Lake Wingra at Madison, Wisconsin.

INTRODUCTION

The problems associated with the eutrophication of lakes and impoundments are becoming of increased concern. One preliminary[1] survey of problem lakes and reservoirs in the U.S. identified numerous cases where the water quality has deteriorated to the extent that restoration measures are needed. Considerable research has been devoted to understanding the role of principal nutrients[2,3,4] in controlling the rate of eutrophication. Particular emphasis has been placed on applying this new knowledge to the development of effective control and restoration measures[5]. Although a wide variety of techniques[6] have been developed, no general guidelines are currently available with which to assess the technical and economic feasibility of alternate techniques. Considering the high costs generally associated with the implementation of lake rehabilitation techniques, there is a great need for reliable predictive tools with which to assess and evaluate the effectiveness of rehabilitation techniques and to estimate the rates of lake recovery. The logical tool which can be used to develop such a predictive capability is mathematical modeling.

In a recent research project[7] for EPA, a general methodology based on the application of modeling techniques was developed for use in assessing the rates of eutrophication in lakes and impoundments. The methodology uses three specific modeling techniques for: (1) estimating nutrient loading rates from land use patterns and historical data[8], (2) predicting the long term changes in key eutrophication indicators as functions of nutrient loading rates[9], and (3) predicting short term changes in several water quality parameters as functions of nutrient loading, climatic conditions, lake morphometry, hydrologic features, thermal and ecologic regimes[10]. In this paper, we present the generalized limnological model developed for short term predictions (less than 10 years) with results from recent applications.

MODELING APPROACH

The conceptual framework of the generalized model is based on a description of the fundamental limnetic processes such as heat transport, constituent transport, hydromechanics, chemical and biological cycles. A quasi-two-dimensional approach is used based on a segment-layer representation shown in Figure 1.

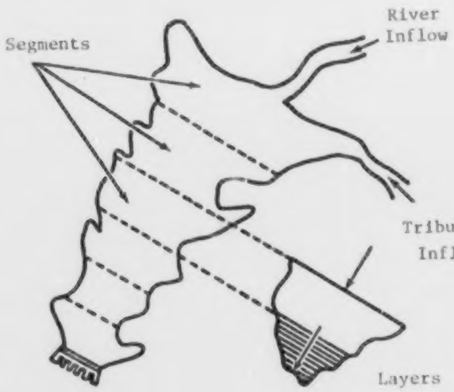

Figure 1. Segment-Layer Representation

This approach reduces the multi-dimensional problem into a series of one-dimensional ones. The fundamental conservation laws for mass and energy are used to derive principal model equations. Chemical and biological cycling are modeled by first order kinetic equations.

TRANSPORT

The heat and mass balance equations for the segment-layer representation are

$$\frac{\partial T}{\partial t} + \frac{Q_v}{A}\frac{\partial T}{\partial z} = D_z \frac{\partial^2 T}{\partial z^2} + \frac{1}{A\Delta z}(Q_{h,i}T_i - Q_{h,o}T) + H \tag{1}$$

and

$$\frac{\partial C^{(k)}}{\partial t} + \left(\frac{Q_v}{A} - v_s\right)\frac{\partial C^{(k)}}{\partial z} = D_z \frac{\partial^2 C^{(k)}}{\partial z^2} + S^{(k)}$$

$$+ \frac{1}{A\Delta z}(Q_{h,i}C_i^{(k)} - Q_{h,o}C^{(1)}) \tag{2}$$

where

T, T_i = lake and inflow temperatures, °C
$C^{(k)}, C_i^{(k)}$ = lake and inflow concentrations, mg/l
$Q_{h,i}, Q_{h,o}$ = horizontal inflow and outflow, m^3/day
Q_v = vertical flow rate, m^3/day
v_s = settling velocity, m/day
$H, S^{(k)}$ = source or sink terms, °C/day, mg/l-day
$A, \Delta z$ = element surface area and thickness, m^2, m

The source terms H account for the atmospheric heat exchanges across the air-water interface and $S^{(k)}$ describes the biogeochemical cycling in the aquatic system. The specific formulations for S are given in the following sections.

DISPERSION AND MIXING

Wind shear on the water surface plays a major role in generating epilimnetic mixing. The following empirical formula is used to calculate vertical dispersion:

$$D_z = a_1 + a_2 v_w e^{-4.6z/d} \qquad (3)$$

where v_w is wind speed, m/sec; d is the depth of the thermocline, m; and a_1 and a_2 are empirical constants, m^2/sec, m. When well-mixed conditions exist, i.e., no thermocline, the depth parameter, d, is set to 6 meters; this represents a minimum stirred depth. Convective mixing produced by density induced instabilities is modeled as a mechanical mixing process. The procedure consists of checking the density profile obtained from the predicted temperatures, locating any region of instability and then mixing the adjacent layers until a stable condition is reached. The outcome of this process is a mixed mean temperature and concentration over the region of instability.

PHYTOPLANKTON

The phytoplankton submodel is based on a carbon balance. A single species formulation is used given by

$$\frac{dP}{dt} = (G_p - D_p)P \qquad (4)$$

where P is the phytoplankton concentration, mg-C/l; G_p is gross specific growth rate, 1/day; and D_p is the death rate, 1/day. The equation for G_p relates the growth rate to the limiting nutrient concentration, light intensity and temperature:

$$G_p = G_m\, G_\ell G_{np} \qquad (5)$$

The term, G_m, is the maximum specific growth rate and is corrected for temperature according to a Q_{10} formula. The light limiting term G_ℓ, is calculated using the equation:

$$G_\ell = \left[\frac{AI}{\sqrt{1 + (AI)^2}}\,\frac{1}{\sqrt{(1 + (\alpha I)^2)}}\right] \qquad (5)$$

where A is a light constant, 1/lux; I is light intensity, lux; and α is a photoinhibition factor, 1/lux. Light intensity is distributed vertically through the water column according to

$$I = I_o\, e^{-(\alpha_o + \beta\bar{P})z} \qquad (7)$$

where I_o is surface light intensity, lux; α_o is extinction coefficient of water, m^{-1}; β is self-shading factor, m^{-1}/mg-C/l; and $\bar{P}$ is average phytoplankton concentration above depth, z, mg-C/l. The diurnal pattern of light is calculated from standard light day equation:

$$I_o = I_{max}\, \tfrac{1}{2}(1 + \cos \frac{2\pi}{\lambda} t) \qquad (-\lambda/2 \leq t \leq +\lambda/2) \qquad (8)$$

where I_{max} is calculated from net short wave radiation; t is time, hours; and λ is the day length factor, hours. The factor, G_{np}, relates the growth rate to the concentration of the principal nutrients:

$$G_{np} = \mathrm{Min}\left[\frac{C_1 + C_3}{(K_n + C_1 + C_3)},\ \frac{D_1}{(K_p + D_1)}\right] \qquad (6)$$

where C_1 and C_3 are ammonia and nitrate nitrogen, mg-N/l; D_1 is inorganic phosphorus, mg-P/l; and K_n and K_p are Michaelis constants.

The decrease in phytoplankton concentration occurs through endogenous respiration, decomposition, sinking, and zooplankton grazing. The formulation for D_p is

$$D_p = \begin{Bmatrix} R_p + C_g Z, & z \leq d_e \\ F_p + C_g Z, & z > d_e \end{Bmatrix} \qquad (9)$$

where R_p is endogenous respiration, 1/day; F_p is decomposition rate, 1/day; C_g is zooplankton grazing, 1/mg-C-day; and d_e is euphotic depth, m. All algal cells within the euphotic zone are treated as active cells which photosynthesize in a lighted environment and respire in a dark one; below the euphotic depth, all algal cell, are inactive cells in the death phase and thus decomposing.

ZOOPLANKTON

The formulation of the zooplankton submodel is given by

$$\frac{dZ}{dt} = (G_z - D_z)Z \qquad (10)$$

where G_z and D_z are the growth and death rates, 1/day.

The zooplankton growth and death rates are calculated from

$$G_z = A_{zp}\, C_g \frac{P}{K_{mp} + P} \qquad (11)$$

$$D_z = R_z + F_z \qquad (12)$$

where A_{zp} is the conversion efficiency, decimal; C_g is grazing rate, 1/day; K_{mp} is Michaelis constant, mg-C/l; and R_z = respiration rate, 1/day; F_z is a predation rate, 1/day. Growth and death rates a corrected for temperature.

PHOSPHORUS

The phosphorus submodel considers algal uptake and release, zooplankton release, degradation of organic phosphorus (D_2) with consequent release of inorganic phosphorus (D_1), loss of both organic and inorganic phosphorus to the sediments (D_3), and anaerobic release from the sediments. The organic phosphorus pool is assumed to be in a particulate form. Settling of particulate P is accounted for in the transport equation. The submodel equations are

$$\frac{dD_1}{dt} = -G_p P A_{pp} + ([I_3 D_3] - I_1 D_1) + I_2 D_2 \qquad (13)$$

$$\frac{dD_2}{dt} = + R_p PA_{pp} + D_z ZA_{pz} - (I_4 D_2) - I_2 D_2 \qquad (14)$$

$$\frac{dD_3}{dt} = + I_1 D_1 + (I_4 D_2 - [I_3 D_3]) \qquad (15)$$

where A_{pp} and A_{pz} are the yield coefficients; I_1 is sediment uptake rate, 1/day; I_2 is organic phosphorus decay, 1/day; I_3 is sediment release, 1/day; and I_4 is sediment trapping, 1/day. The terms in parenthesis apply for the hypolimnion; brackets designate processes dependent on anaerobic conditions. The rate coefficient I_1, I_2, I_3 and I_4 are corrected for temperature.

NITROGEN

The nitrogen submodel considers algal uptake and release, zooplankton release, decay of organic (C_4) and sediment (C_5) nitrogen, and the oxidation of ammonia (C_1) and nitrite (C_2) to nitrate (C_3). During anaerobiosis, nitrification is inhibited and denitrification occurs with the loss of nitrate. Sediment interactions include nitrate uptake and release of ammonia. The organic nitrogen pool is assumed to be in particulate form; settling of particulate N is accounted for in the transport equation. The submodel equations are

$$\frac{dC_1}{dt} = - J_1 C_1 - PG_p A_{NP} \frac{C_1}{C_1 + C_3} + J_4 C_4 + (J_5 C_5) \qquad (16)$$

$$\frac{dC_2}{dt} = J_1 C_1 - J_2 C_2 \qquad (17)$$

$$\frac{dC_3}{dt} = J_2 C_2 - PG_p A_{NP} \frac{C_3}{C_1 + C_3} - J_3 C_3 \qquad (18)$$

$$\frac{dC_4}{dt} = J_4 C_4 + R_p PA_{NP} + D_z ZA_{NZ} - (J_6 C_4) \qquad (19)$$

where J_1 is the ammonium oxidation rate, 1/day; J_2 is nitrite oxidation rate, 1/day; J_3 is denitrification rate constant, 1/day; J_4 is organic nitrogen decay, 1/day; J_5 is sediment nitrogen decay, 1/day; J_6 is sediment uptake rate, 1/day; and A_{NP} and A_{NZ} are the nitrogen to carbon ratios for algae and zooplankton, mg-N/mg-C. Denitrification is inhibited during aerobic conditions. The rate coefficients J_1, J_2, ..., J_5 are adjusted for temperature.

BIOCHEMICAL OXYGEN DEMAND

The behavior of BOD is modeled by

$$\frac{dL_c}{dt} = - K_1 L_c + a_o (F_p P + R_z Z) \qquad (20)$$

where L_c is the BOD_5 concentration, mg/l, K_1 is the decay rate, 1/day, and a_o is a stoichiometric constant, mg-O_2/mg-C.

DISSOLVED OXYGEN

The dissolved oxygen submodel considers the effects of (1) temperature, (2) oxidation of suspended and dissolved organic matter, (3) benthic uptake, (4) reaeration, (5) algal photosynthesis, respiration and decomposition:

$$\frac{dDO}{dt} = - K_1 L_c - a_1 J_1 C_1 - a_2 J_2 C_2 - \frac{L_b}{\Delta z} + K_r (DO_s - DO)$$
$$+ a_3 (G_p - D_p) P \qquad (21)$$

where DO_s is dissolved oxygen saturation, mg/l; L_b is benthic oxygen uptake rate, g/m^2-day; a_1, a_2 and a_3 are stoichiometric constants; and K_r is reaeration coefficient 1/day. All other variables are as previously defined.

A simple linear relationship is used to model reaeration rate as functions temperature and wind speed:

$$K_r = (a_1 + a_2 v_w) \theta^{(T-20)} \qquad (22)$$

where v_w is wind speed, m/day; a_1 and a_2 are empirical coefficient; and T is temperature in °C. θ is 1.075.

MODEL APPLICATIONS

The chemical and biological submodels described above have been implemented into a generalized computer model. The simulation procedure for a general application consists of two steps. First, the heat transport, mixing and fluid flow are simulated for the entire period of interest using 1 day time steps. Next, these results are input to the limnological model for solution of the equations for constituent transport, which are solved, using 4 to 12 hour time steps, for each of 11 constituents. A finite difference technique is used to obtain approximate solutions for the transport equations.

LAKE WASHINGTON

Lake Washington is a large, relatively deep, mesotrophic lake located at Seattle, Washington. The pollution history and recovery of the lake has become a classic example of how a eutrophic lake can show a positive response to nutrient diversion. Because of the lake's depth and aerobic environment, the lake lacks significant sediment-water interactions. Consequently, Lake Washington is a good case for testing a model's ability to describe the transport of dissolved and particulate matter, nutrient cycling and algal growth patterns as they are influenced by the annual stratification cycle.

The limnological model was applied for the time period April 1 through December 31, 1962. This period was selected because it represented that portion of the year over which the chemical and biological changes were most dynamic. A single segment with 20 elements was used to represent the lake geometry. The inflow quality data for the lake were adapted from estimates developed by Chen[1] in a previous modeling effort. The model results are compared with observed data in Figure 2. The good-to-excellent agreement of these results indicate the model has a strong capability to describe the direct and reciprocal relationships between algae dynamics and nutrient cycling. Calibration of the temperature model required about 10 minutes computer time, on a PDP 11/45, and 30 minutes of staff time. The limnological model required about 1 hour of computer and staff time to calibrate.

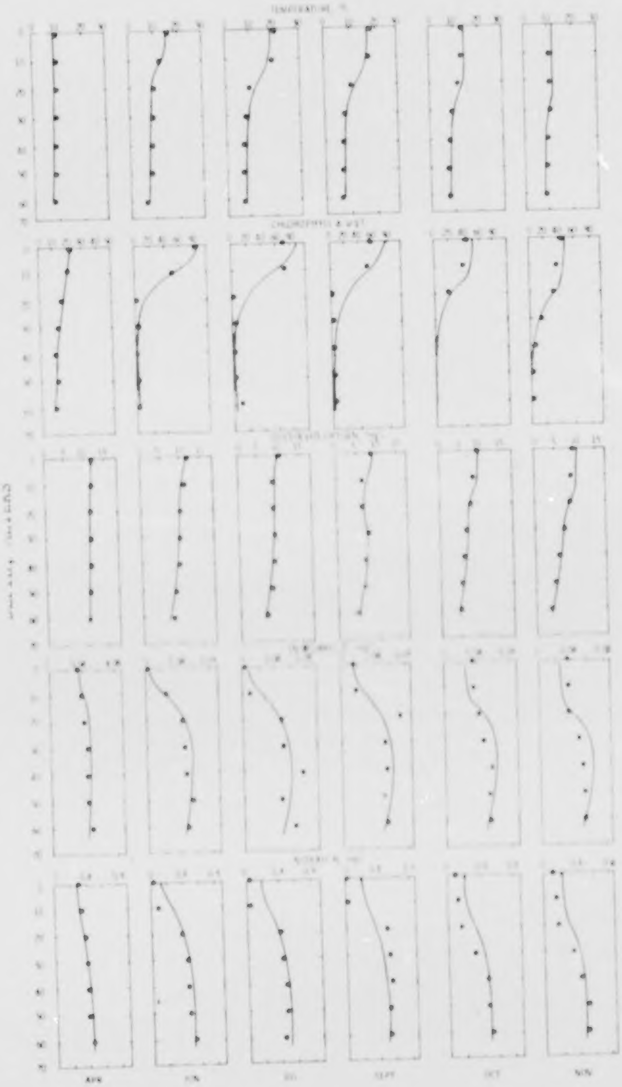

FIGURE 2. Lake Washington Application

LAKE MENDOTA

Lake Mendota is a large, moderately deep, eutrophic lake located at Madison, Wisconsin. The largest of the Madison lakes, it enjoys the notable distinction of being one of the most studied and well characterized lakes in the world. The limnological patterns in the lake are very diverse and complex. The phytoplankton cycle is characterized by a species succession typical of eutrophic lakes. The nutrient cycles are very dynamic and strongly related to the phytoplankton and dissolved oxygen cycles. Thus, Lake Mendota represents a considerable challenge for any limnological model.

The model was applied to Lake Mendota for the period from May 8 through October 18, 1972. The major chemical and biological transformations occur within this period. Considerable in-lake data[12] are available for the lake. The inflow quality was estimated from data compiled by Sonzogni and Lee.[13] The lake was represented by a single segment with 16 layers. The model results are compared with the observed data in Figure 3. These results clearly show that the model has a strong capability to track the algal growth and nutrient cycling patterns in stratified lakes with sediment interactions and anoxic regimes. These results further demonstrate that the model can realistically relate the biological, chemical and physical response of the lake to major controlling factors. The model produced excellent results for temperature, chlorophyll a, inorganic phosphorus, and ammonia nitrogen. Good-to-excellent results for dissolved oxygen were obtained. The results for nitrate nitrogen indicate that additional development work is needed to improve the nitrogen submodel.

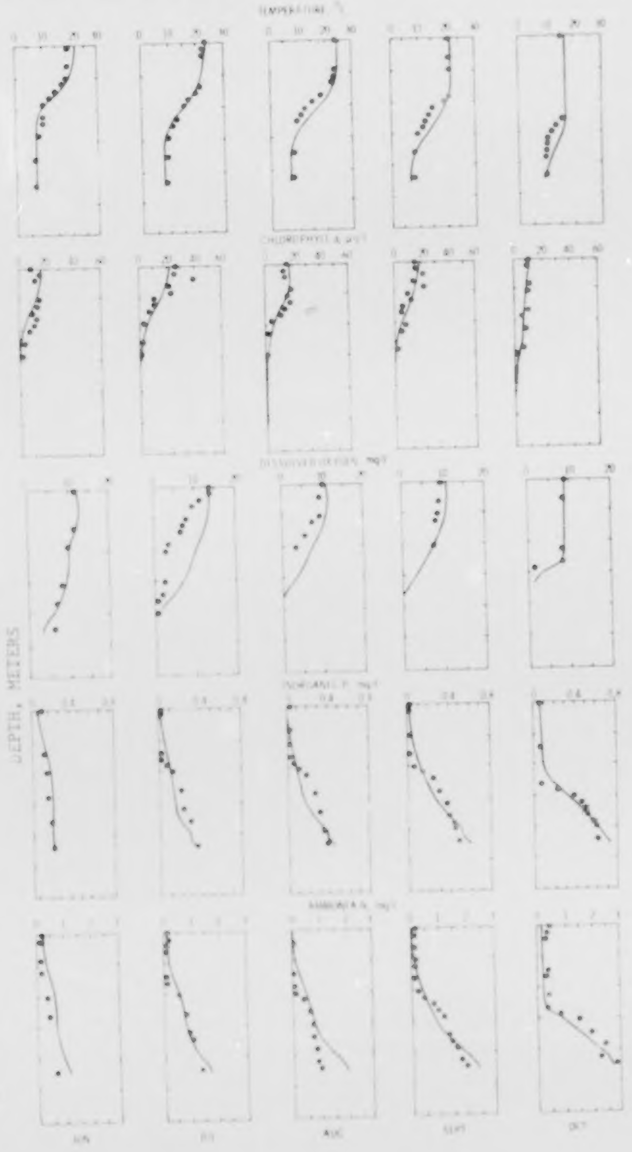

FIGURE 3. Lake Mendota Application

LAKE WINGRA

Lake Wingra is a small shallow lake located near the university of Wisconsin at Madison. The lake is presently in an advanced eutrophic state. Because the lake receives its nutrients from intermittent sources (precipitation, dry fallout, urban and rural runoff) the net loading rate history resembles a high frequency random signal. The instantaneous flushing rate also varies from a few weeks to several months. The net result is that the chemical and biological state of the lake are very sensitive to the boundary conditions during certain parts of the year.

The limnological model was applied for the time period April 1 through October 31, 1970. Inflow quality data were developed from measurements reported by Kluesener[14] and estimates of diffuse inputs (dry fallout, rainfall). The in-lake data collected Kluesener[14] and Koonce[15] were used for initial conditions and the model comparison. A single segment representation composed of six layers was used. The comparisons between the in-lake data and the model results show good agreement for most water quality parameters. Temperature and dissolved oxygen were modeled exceptionally well. Since the biomass data were calculated from cell counts and volumes there are some questions about the comparability of the phytoplankton biomass results. Nevertheless, the model results are quite reasonable and show the proper relationship between parameters.

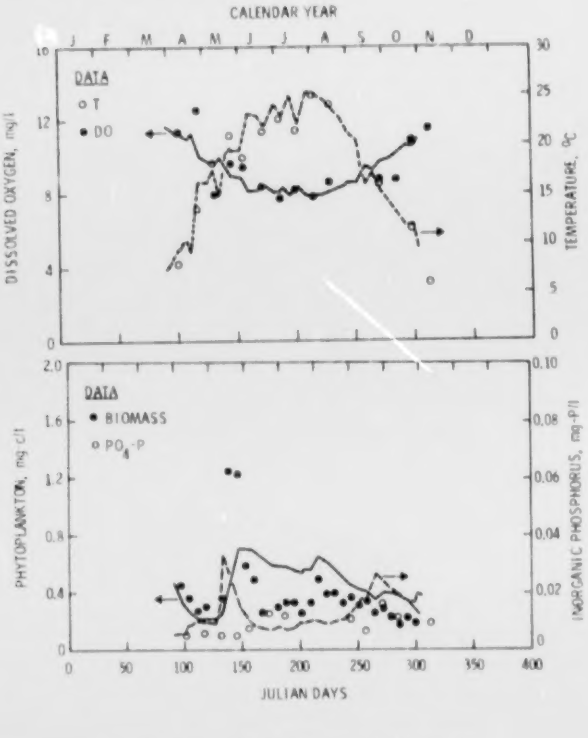

FIGURE 4. Lake Wingra Application

CONCLUSIONS

The general capability of the models developed in this work has been demonstrated with applications to three lakes: Lake Washington at Seattle, Lakes Mendota and Wingra at Madison, Wisconsin. These three lakes represent a class of eutrophic lakes with different morphometric, meteorologic, hydrologic, thermal, and ecologic regimes. The comparisons between observed data and model results demonstrate that the models have a general capability to track the seasonal water quality patterns in limnetic systems.

The generalized limnological model presented in this paper can provide a convenient interpretative tool and can be used to develop an understanding of the limnetic system as a whole. By providing information on the cause and effect relationships, these models can help expand our insight and improve our abilities to predict the ecological consequences of altering various controlling factors.

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MATHEMATICAL MODELING OF PHYTOPLANKTON DYNAMICS IN SAGINAW BAY, LAKE HURON

V. J. Bierman, Jr.
U.S. Environmental Protection Agency
Large Lakes Research Station
Environmental Research Laboratory-Duluth
Grosse Ile, Michigan

D. M. Dolan
U.S. Environmental Protection Agency
Large Lakes Research Station
Environmental Research Laboratory-Duluth
Grosse Ile, Michigan

Summary

A mathematical model of phytoplankton production has been applied to a set of physical, chemical, and biological data from Saginaw Bay, Lake Huron. The model includes five phytoplankton types, two zooplankton types, and three nutrients: phosphorus, nitrogen, and silicon. The phytoplankton types include diatoms, greens, both nitrogen-fixing and non-nitrogen fixing blue-greens and "others".

The purpose of the paper is to illustrate the use of the model in both research and management applications. A major research use to be discussed is the interpretation of experimental data. An example is the calibration of model output for total phosphorus concentration to actual field data. This calibration indicated the possibility of a previously unconsidered phosphorus source influencing the bay in the fall of 1974.

An important management application of the model is its use as a tool for comparing the effects of various wastewater management strategies. An example is the simulation of differences in response among the various phytoplankton types as a function of nutrient load reduction in Saginaw Bay. These examples and others are discussed in this paper.

Introduction

Mathematical modeling techniques can provide a quantitative basis for the comparison of various management strategies designed to reduce waste loadings to receiving bodies of water. Different management strategies for the Great Lakes have been analyzed in this manner. Thomann, et al. have used these techniques to investigate the effects of phosphorus and nitrogen reduction on chlorophyll levels in Lake Ontario.[1] Bierman, et al. have investigated the effects of changes in phosphorus, nitrogen, and silicon loadings on phytoplankton biomass in Saginaw Bay, Lake Huron.[2]

Exhaustive research must be conducted with mathematical models prior to their use as management tools, to ensure that they accurately describe the particular physical, chemical and biological processes that they were designed to simulate. Canale and Middlebrooks, et al. have reported on various research oriented whole-system and component models which were designed to obtain greater insight with regard to chemical and biological processes in aquatic ecosystems.[3,4]

The present work is part of the International Joint Commission's Upper Lakes Reference Study involving Saginaw Bay, Lake Huron. The ultimate goal of this work is to develop a mathematical model which can be used both to describe the physical, chemical and biological processes that occur in Saginaw Bay and to predict the effects of reduced waste-loadings.

Model development is proceeding along two parallel pathways. The first of these involves the development of research-oriented process models which include biological and chemical detail but which, for simplicity, do not include any spatial detail. The second pathway involves the development of an engineering-oriented water quality model which describes, as closely as possible, the actual physical system, including spatial detail. At any point in time, the water quality model will simulate those chemical and biological processes which have been successfully investigated and developed using the spatially-simplified model. There is constant feedback between the above two pathways and constant interaction between the entire modeling effort and an ongoing sampling program on Saginaw Bay.

The purpose of the present paper is to describe the basic concepts of the Saginaw Bay model and to present sample output from the model which illustrates its use both as a research tool and as a management tool. All reported results were obtained using a spatially-simplified model applied to the inner portion of Saginaw Bay (Figure 1), which has been assumed to be a completely-mixed reactor.

Model Concepts

The basic model equations and preliminary simulations appear elsewhere.[5,6] The compartments in the model are five phytoplankton, two zooplankton, higher predators, and three nutrients: phosphorus, nitrogen, and silicon (Figure 2). The phytoplankton types are diatoms, greens, both nitrogen-fixing and non-nitrogen-fixing blue-greens, and "others", mostly dinoflagellates and cryptomonads in Saginaw Bay.

The motivation for a multi-class modeling approach is that different classes of algae have very different nutrient requirements; for example, diatoms have an absolute requirement for silicon and certain types of blue-greens can fix atmospheric nitrogen. In addition, not all of these classes have the same nuisance characteristics. Diatoms and green algae are grazed by zooplankton, but blue-green algae are not significantly grazed and can form objectionable floating scums.

A unique feature of the model is that cell growth is considered to be a two-step process involving separate nutrient uptake and cell synthesis mechanisms. The motivation for this variable stoichiometry approach is that an increasingly large body of experimental evidence indicates that the mechanisms of nutrient uptake and cell growth are quite distinct.[7,8,9,10,11] The model includes carrier-mediated uptake of phosphorus and nitrogen using a reaction-diffusion mechanism, and possible intermediate storage in excess of a cell's immediate metabolic needs. Specific cell growth rates are assumed to be dependent on the intracellular levels of these nutrients, in contrast to the use of Michaelis-Menten equation for relating growth rates directly to extracellular nutrient concentrations.

Model Implementation

A major problem in attempting to implement a complex chemical-biological process model is the lack of sufficient experimental data. It is often possible that more than one set of model coefficients could produce acceptable agreement between the model output and a given data set. In the transition from single-class to multi-class models, this problem becomes particularly acute because it is no longer sufficient to ascertain a range of literature values for a given coefficient. Multi-class models necessitate the definition of class distinctions within this range. Given the present state of the art of ecosystems modeling and associated experimental work, many of the coefficients in such models must simply be estimated.

The primary operational differences among the phytoplankton types in the model are summarized in Table 1. The working equations of the model and sensitivity analyses of some of the more important coefficients have been presented elsewhere.[5]

One of the implicit assumptions of the model is that cell biomass concentration is a more accurate indicator of phytoplankton standing crop than is chlorophyll a concentration. Furthermore, chlorophyll a is a lumped parameter and cannot be used to distinguish between different functional groups of phytoplankton. For these reasons, chlorophyll a concentration does not appear in any of the kinetic equations of the model.

The computer program which actually solves the model equations is written in FORTRAN IV and is structured in a form such that any number of phytoplankton and zooplankton types can be simulated, along with any set of food web interactions for these groups. The version of the model in Figure 2 consists of 23 simultaneous differential equations. The solutions were obtained using a fourth-order Runge-Kutta method with a time step of 30 minutes for the nutrient kinetics equations and a time step of 3 hours for the growth equations. For a 365-day simulation, approximately 5 minutes of CPU time are required on an IBM 370/158 computer. For the same simulation, approximately 60 minutes of CPU time is required on the Grosse Ile Laboratory's PDP-8/e minicomputer with floating point hardware.

Experimental Data

Chemistry and chlorophyll data were collected for Saginaw Bay by Cranbrook Institute of Science.[12] During 1974, 12 cruises were conducted and samples were collected from 59 stations. Samples were taken at 1 meter and at all depths from 5 meters to the bottom in 5-meter intervals. A total of 111 station-depth combinations were sampled on most of the cruises. Analyses were conducted for 21 chemical parameters, including phytoplankton chlorophyll. Since the present modeling study is restricted only to the inner portion of Saginaw Bay (Figure 1), only data from the 33 field stations in this region were used.

The phytoplankton data used were collected on the above cruises by the University of Michigan at 1 meter depths.[13] Species counts were conducted on all samples. In order to transform these data for comparison with model output, the species counts were first integrated to the genus level. At this level, cell volumes were assigned and these volumes were then integrated to the level of the five functional groups in the model. The cell volume concentrations at this level were converted to dry weight (biomass) concentrations.

The zooplankton data used were collected on the above cruises by the University of Michigan at the same station-depth combinations as the chemical data.[14] Individual species counts were converted directly to dry weight concentrations and then integrated to the level of the two functional groups in the model.

All phytoplankton and zooplankton mean concentrations are reported as the geometric mean ± 34% of the area under the frequency distribution curve. This is analogous to the arithmetic mean ± one full standard deviation. Analyses of the biological data indicated that a log-normal distribution was a more accurate representation than a normal distribution. All other data are reported as the arithmetic mean ± one-half standard deviation.

Nutrient loadings to Saginaw Bay from the Saginaw River, the primary source, were determined on the basis of a field sampling program. For the first half of the year, samples were taken at two to three-day intervals at the Dow Chemical Company water intake at the mouth of the Saginaw River. From July to December, samples were taken from the Midland Street Bridge in Bay City every two weeks. During this period, the Dow intake was too strongly influenced by the bay itself because of the intrusion of bay water up the river. The Midland Street Bridge is approximately 5 miles upstream from the river mouth and is not influenced by the bay during this period. Concentrations were obtained for chloride and total and dissolved forms of phosphorus, nitrogen, and silicon. Daily flow rates were obtained from the U.S. Geological Survey.

Boundary Conditions and Forcing Functions

Since the physical system under consideration is only part of a larger physical system, Lake Huron proper, the interaction between Saginaw Bay and Lake Huron is extremely important. The predominant flow pattern in the bay is counterclockwise with Lake Huron water flowing in along the north shore and a mixture of Lake Huron water and Saginaw River water flowing out of the bay along the south shore (Figure 1). The concentrations of nutrients and biota in the water which flows across the indicated inner bay-outer bay boundary are examples of boundary conditions which must be specified. These concentrations were determined using the cruise data from the two sampling stations nearest to the area of water inflow from the outer bay. Daily concentration values were calculated by linearly interpolating between the cruise averages for these stations.

External nutrient loads are the most important forcing functions in the present study. Total daily flow from the Saginaw River was calculated by summing the primary tributary gauges and the estimated flow from the ungauged tributary area. Daily nutrient loading rates were calculated using the measured nutrient concentrations on that day. These daily loading rates were then plotted and time-series of loading rates were generated by linearly interpolating between all of the significant peaks and troughs. For example, for total phosphorus, a series of 28 loading rates/time-breaks was generated. For orthophosphorus, a series of 46 loading rates/time-breaks was generated.

Model Calibration

The spatially-simplified Saginaw Bay model has been calibrated to 12 simultaneous and independent parameters: chloride, biomass concentrations for five functional groups of phytoplankton, total zooplankton, total phosphorus, total nitrogen, and dissolved forms of phosphorus, nitrogen, and silicon. For simplicity, only selected results are presented here (Figures 3-5).

Water circulation rates between the inner and outer bay were determined by modeling chloride concentrations in the bay and chloride loadings from the Saginaw River in a manner similar to that of Richardson.[15] Advective flows and turbulent dispersions in the model were adjusted until the chloride output corresponded to the field measurements (Figure 3). Time-variable flows were used which corresponded to hydraulic detention times ranging from 45 to 120 days for the inner bay.

Model output for total phosphorus (Figure 4) is consistent with the actual data with the exception of the late-fall period. Since the only external nutrient sources considered were the Saginaw River and Lake Huron, the present results must be considered preliminary in nature. The possible roles of sediments and atmospheric sources must be considered before a complete picture of the nutrient dynamics in Saginaw Bay can be obtained.

One of the recent advances in the area of phytoplankton modeling has been the resolution of total phytoplankton biomass into functional groups. There are important differences in biology and nutrient chemistry among different types of algae, as well as differences in water quality implications. In Saginaw Bay, the principal concern is with the differences between diatoms and blue-green algae. The total biomass curve (Figure 5) was therefore resolved into its diatom and blue-green components (Figure 6) by plotting the computed biomass concentrations of these phytoplankton types. Comparison of the curves indicates that the diatoms (Figure 6a) comprise 99% of the first biomass peak, while the sum of non-heterocystous blue-greens (Figure 6b) and hetercystous blue-greens (Figure 6c) comprises 80% of the second biomass peak. The results agree reasonably well with biomass data for individual phytoplankton types.

Research Applications

The present model can be applied to a variety of research problems. It can be an extremely useful research tool when used in numerical experimentation or sensitivity analyses. Those system parameters which are sensitive over the range of interest can be identified. Given a limited research budget, the information can be useful in optimally directing spending. The model provides an alternate framework for data analysis which can supplement traditional methods such as statistical summaries or empirical models. Use of the model can lead to new interpretations of existing data or make clear new data requirements.

The total phosphorus calibration (Figure 4) provides a good example of the model providing a framework within which to interpret data. The calculated phosphorus concentration in the 4th quarter is consistently low when compared to the actual data. This indicates that an additional total phosphorus source is probably influencing the system in the fall and that this source is not included among the model inputs. In support of this hypothesis, the calculated phosphorus concentrations agree quite well with observed data in the other parts of the year and the calculated chloride concentrations and hence, water circulation rates agree with the observed data over the entire year. Phosphorus sources thought to be insignificant on an annual basis have been reconsidered for possible seasonal inputs. Such sources include contributions from the atmosphere, resuspension of sediments and possible leaching from dredge spoils. This apparent discrepancy could not have been discovered by looking at total phosphorus loadings and open-water concentrations alone. The model provides a link between the two that allows such a conclusion to be made.

Additional research insight can be gained by the resolution of total phytoplankton biomass into various functional groups. With this increased resolution, the full range of phytoplankton-nutrient interactions can be investigated including:

1. nutrient recycling among different functional groups,
2. differences in nutrient stoichiometries and kinetics among the functional groups,
3. effect of silicon and nitrogen on species composition and succession,
4. supply of nitrogen to the system by nitrogen fixing blue-green algae.

Research with a sophisticated mathematical model requires the investigator to consider new data and to reconsider existing data. Explanation of previously undiscovered phenomena now becomes necessary. Also, as the model attains more realism, empirical coefficients and constants are eliminated and experimentally determined parameters take their place. Some examples follow.

Chlorophyll a concentrations in water are relatively easy to determine. In conventional chlorophyll models, the chlorophyll a to biomass ratio for phytoplankton is assumed to be constant. Chlorophyll a concentrations are therefore taken to be adequate measures of phytoplankton abundance. However, when actual biomass data were collected for calibration of the multi-class model in Saginaw Bay, the chlorophyll a to biomass ratio was found to vary over the year by as much as a factor of 16. Furthermore, these data indicated that the chlorophyll a to biomass ratio changed as phytoplankton species succession occurred throughout the year. This observation suggested that each functional group in the model should have a distinct chlorophyll a to biomass ratio, and that the overall ratio at any given time depends on the relative abundance of each of the functional groups. Assigning chlorophyll a to biomass ratios by phytoplankton group reduced significantly the yearly variation in the overall chlorophyll a to biomass ratio.

Field data alone cannot provide information needed to replace empirical coefficients in simpler models. The development of the model has necessitated comprehensive process-rate studies to determine phytoplankton-nutrient uptake kinetics, as well as phytoplankton-zooplankton interactions. These types of process studies have value independent of their modeling utility, but the modeling process can assure that they are conducted in an orderly fashion.

Management Applications

A model that has been rigorously calibrated and verified can be used for planning and management purposes. The achievement of significant reductions in algal biomass, especially nuisance blue-greens, is a problem that the multi-class phytoplankton model is uniquely qualified to address. The problem can be quantified by introducing the possibility of reductions in the key nutrients: phosphorus, nitrogen and silicon in the case of Saginaw Bay. The model is capable of predicting reductions in each class of algae given a percent reduction in the loadings of these three nutrients. It should be emphasized that, in practice, such reductions would have to be accomplished by consideration of the controllable portion of each of the nutrient loads, the timing of the loadings and the availability of each nutrient to the algae.

Although, in the strict sense, the present model is not verified, hypothetical simulations were conducted in which the external loads of phosphorus, nitrogen and silicon, respectively, were reduced by 50%. The effect of a 50% reduction in nitrogen loadings was found to have a negligible effect on algal biomass. This is not surprising because nitrogen is abundant in Saginaw Bay at the time of the spring diatom bloom and nitrogen-fixing blue-greens can make up any deficit in the supply of dissolved nitrogen later in the season. A 50% reduction in silicon loading was found to cause a minor reduction in the diatom crop. Silicon reductions were less effective than expected because zooplankton grazing is apparently as important as silicon depletion in the termination of the spring diatom bloom. In addition, a large amount of silicon enters the bay from Lake Huron.

Two sets of boundary conditions were considered for the simulation of 50% reduction in phosphorus loadings. In the worst case situation, it is assumed that the outer bay phosphorus concentration remains the same despite the phosphorus load reduction. In the best case situation, it is assumed that the outer bay phosphorus concentration becomes similar to the Lake Huron phosphorus concentration in response to the phosphorus load reduction. The actual "state of nature" will lie within these two extremes. Such an approach is necessitated by the lack of spatial resolution in the present model. With spatial resolution, the outer bay could be modeled also. Thus the ambiguity in boundary conditions would be removed since the system boundary would be Lake Huron which has well defined concentrations for the parameters of interest.

The reduction in algal biomass for the 50% phosphorus load reduction occurs primarily in the latter half of the year. Therefore, it is essentially a reduction in blue-greens, since 80% of the second biomass peak is blue-green biomass. Actual percent reduction in total blue-green biomass depends on the specification of the boundary conditions (Figure 7). The best case blue-green reduction (Figure 7b) is 73% of the peak biomass, while the worst case reduction (Figure 7a) is 26% of the peak biomass. Improved estimates of blue-green responses to waste load reductions in Saginaw Bay can only be obtained with a spatially segmented version of the model.

Nutrient reduction simulations can be used by managers and planners to decide which nutrient or nutrients to focus on in reduction programs and how much reduction in the nutrient is required for significant improvements in water quality.

Future Research

Near term research with the model has two important goals: calibration of a spatially refined model to 1974 data and verification of this model with 1975 data.

A 5-segment version of the model has been developed and is awaiting calibration. The additional spatial resolution will allow examination of effects in different areas of the bay and will reduce the dependence of future projections of water quality on boundary conditions.

Additional spatial resolution depends on adequate representation of the water movement between spatial segments of the model. Work is underway on a hydrodynamic model that will be compatible with the phytoplankton model and will specify the transport on a time varying basis when given wind speed and directions as input.

Longer term goals for Saginaw Bay include the monitoring of water quality trends in the bay as nutrient loadings decrease. During the next several years nutrient reductions are expected to occur due to ongoing abatement programs. Actual projections made with the model indicate that significant improvements in water quality will occur as these reductions are attained. The Saginaw Bay sampling program should detect these trends and thus provide an opportunity for model verification.

This modeling effort has, in addition, some broader, user oriented goals. The phytoplankton model will be tested on other physical systems to determine its generality and to obviate any unforeseen difficulties which might be experienced. An ultimate goal is to transfer a documented version of the model to interested users for research, planning, and management purposes.

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TABLE 1

Operational Differences Among
Phytoplankton Types

Characteristic Property	Diatoms	Greens	Others	Blue-Greens (non n-fixing)	Blue-Greens (n-fixing)
Nutrient Requirements	Phosphorus Nitrogen Silicon	Phosphorus Nitrogen	Phosphorus Nitrogen	Phosphorus Nitrogen	Phosphorus
Relative Growth Rates Under Optimal Conditions	High	High	Low	Low	Low
Saturation Light Intensity	High	High	High	Low	Low
Sinking Rate	High	High	High	Low	Low
Grazing Pressure	High	High	None	None	None

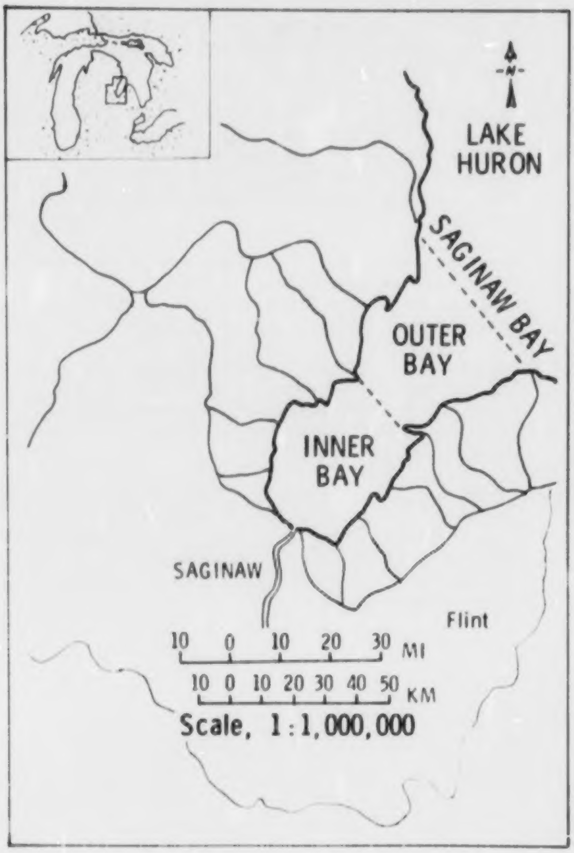

LAKE HURON
SAGINAW BAY
OUTER BAY
INNER BAY
SAGINAW
Flint
N
10 0 10 20 30 MI
10 0 10 20 30 40 50 KM
Scale, 1:1,000,000

Figure 1. Saginaw Bay watershed indicating distinctions between inner and outer portions of the bay.

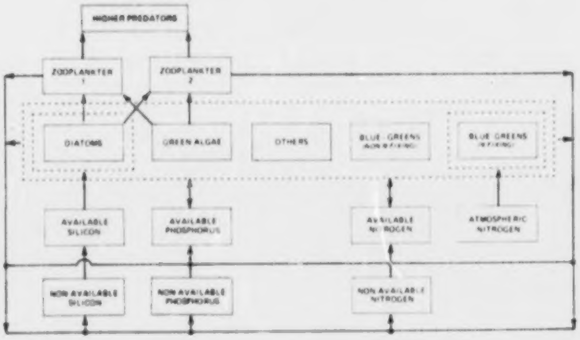

HIGHER PREDATORS
ZOOPLANKTER 1
ZOOPLANKTER 2
DIATOMS
GREEN ALGAE
OTHERS
BLUE GREENS (NON N FIXING)
BLUE GREENS (N FIXING)
AVAILABLE SILICON
AVAILABLE PHOSPHORUS
AVAILABLE NITROGEN
ATMOSPHERIC NITROGEN
NON AVAILABLE SILICON
NON AVAILABLE PHOSPHORUS
NON AVAILABLE NITROGEN

Figure 2. Principal compartments of the Saginaw Bay, inner portion, as compared to model ouput.

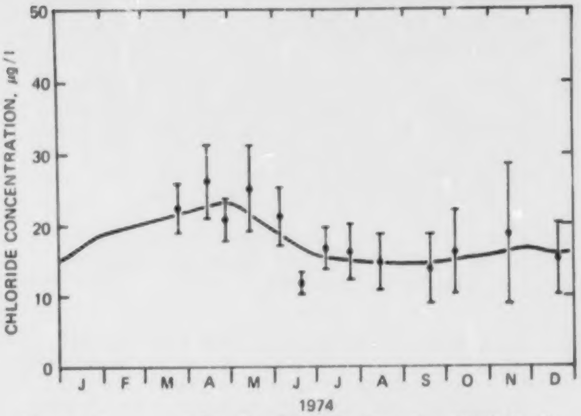


Figure 3. Chloride distribution for 1974 in Saginaw Bay, inner portion, as compared to model output.

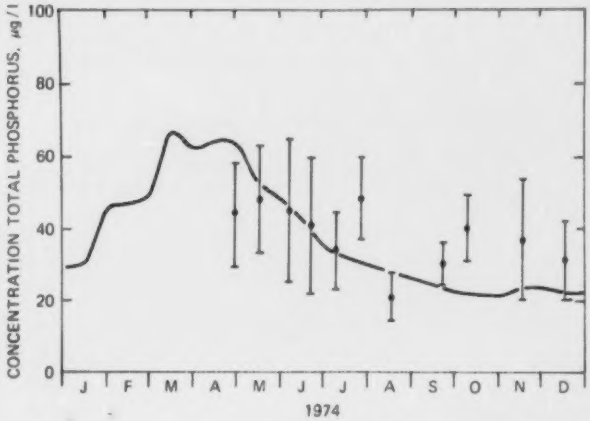


Figure 4. Total phosphorus distribtution for 1974 in Saginaw Bay, inner portion, as compared to model output.

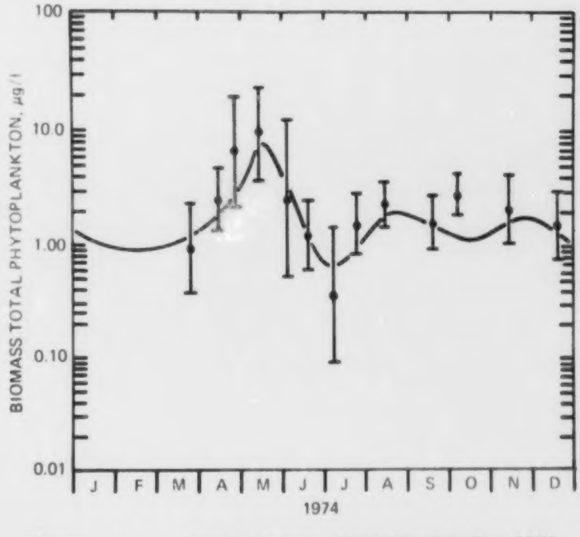


Figure 5. Total biomass distribution for 1974 in Saginaw Bay, inner portion, as compared to model output.

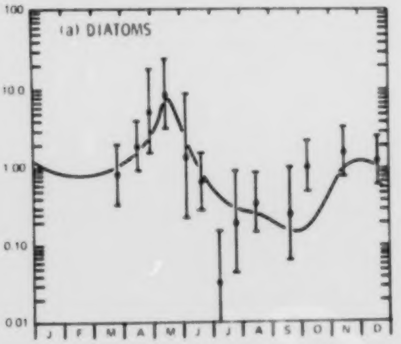


Figure 6(a). Diatom biomass distribution for 1974 in Saginaw Bay, inner portion, as compared to model output.

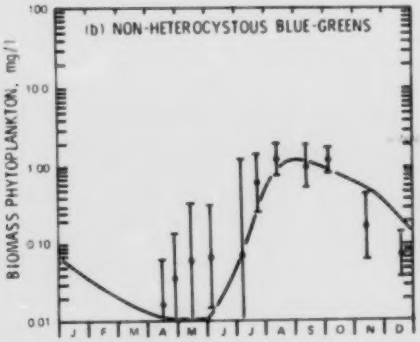


Figure 6(b). Biomass distribution of non-heterocystous blue-green algae for 1974 in Saginaw Bay, inner portion, as compared to model output.

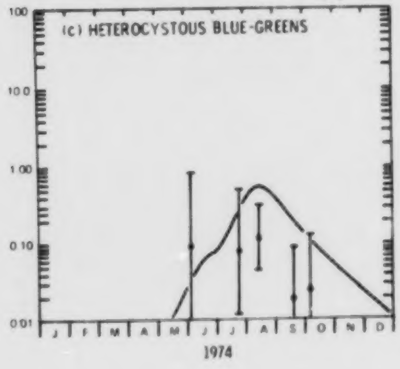


Figure 6(c). Biomass distribution of heterocystous blue-green algae for 1974 in Saginaw Bay, inner portion, as compared to model output.

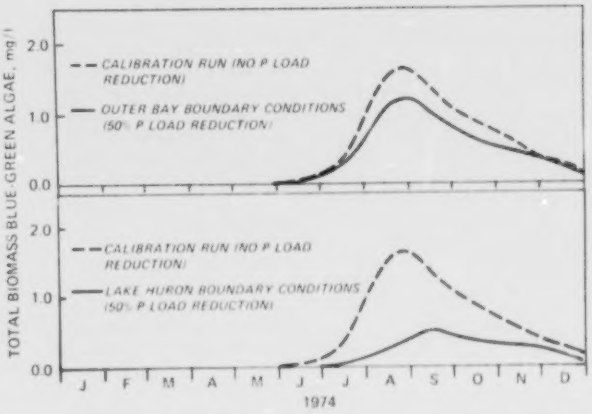


Figure 7(a). Comparison between calibration run and 50% P load reduction simulation for blue-green biomass in Saginaw Bay with outer bay boundary conditions.

THE APPLICATION OF A STEADY-STATE WATER QUALITY MODEL TO THE PERMIT WRITING PROCESS, LAKE MILNER, IDAHO

John R. Yearsley
EPA Region X
Seattle, Washington 98101

SUMMARY

The Milner Reach of the Snake River, between Minidoka Dam and Milner Dam (see Figure 1), is classified as being water quality limited. One of the important limiting water quality parameters is dissolved oxygen. Data collected by the Federal Water Quality Administration (FWQA) and the Environmental Protection Agency (EPA) at Milner Dam show extended periods of low dissolved oxygen. Conditions have been particularly critical during periods of low flow when the discharges from municipal and industrial waste sources were at their peak. For example, during November, 1969 the minimum dissolved oxygen was less than 6.0 mg/l on twenty-three days. The effects of low dissolved oxygen upon aquatic life have reached serious proportions. Major fish kills occurred in the Milner Reach during the 1960, 1961, and 1966 food processing seasons. In addition to the discharge of organic wastes from industrial and municipal sources, the oxygen demand associated with return flow from irrigation wasteways, decay of algae in impoundments and oxygen demand from bottom sediments contribute to the observed dissolved oxygen problems.

Reductions in waste discharge since 1971, coupled with above-average flows in the Snake River, have resulted in substantial improvement in the dissolved oxygen of the Milner Reach. No dissolved oxygen levels below 6.0 mg/l have been observed since 1971. However, dissolved oxygen levels below 90% saturation were measured during the food processing seasons of 1973 and 1974.

In October, 1974, the Idaho Operations Office of the EPA Region X drafted National Pollutant Discharge Elimination System (NPDES) permits for the industrial waste sources, J. R. Simplot and Ore-Ida, in the Burley-Heyburn area. A steady-state dissolved oxygen model was used to support the permit writing process. At the same time, a comprehensive field study program was designed to verify the model results in the Milner Reach.

METHOD OF ANALYSIS

The steady state dissolved oxygen budget for a vertically and laterally well mixed stream, in which diffusion and dispersion processes are neglected, can be written:

$$u \frac{dC}{dx} = -K_2(C - C_S) - K_1 L + \Phi_C - \Gamma_C \qquad (1)$$

where,

u = the stream velocity, feet/second,
C = the dissolved oxygen, mg/l,
x = the distance along the axis of the river, positive downstream, feet,
K_2 = the reaeration rate, 1/days,
C_S = the saturation dissolved oxygen, mg/l,
K_1 = the deoxygenation rate, 1/days,
L = the carbonaceous biological oxygen demand (BOD), mg/l,
Φ_C = the dissolved oxygen sources, mg/l/second
Γ_C = the dissolved oxygen sinks, mg/l/second.

Similarly, the BOD budget is:

$$u \frac{dL}{dx} = -K_1 L + \Phi_L - \Gamma_L \qquad (2)$$

where,

Φ_L = the BOD sources, mg/l/second,
Γ_L = the BOD sinks, mg/l/second,

In the initial permit analysis, the only dissolved oxygen sources considered were those associated with surface and groundwater return flow. The only dissolved oxygen sink was the demand associated with bottom sediments.

Sources of BOD were associated with surface and groundwater return flows, and municipal and industrial discharges. No BOD sinks were included.

The solutions to Equations (1) and (2) are, respectively:

$$C = C_S - (C_S - C_0)\, e^{\frac{-K_2 x}{u}} - \frac{K_1 L_0}{(K_2 - K_1)}\left(e^{\frac{-K_1 x}{u}} - e^{\frac{-K_2 x}{u}}\right) + (\Phi_C - \Gamma_C)\left(\frac{1 - e^{\frac{-K_2 x}{u}}}{K_2}\right) \qquad (3)$$

and,

$$L = L_0\, e^{\frac{-K_1 x}{u}} + (\Phi_L - \Gamma_L)\left(\frac{1 - e^{\frac{-K_1 x}{u}}}{K_1}\right) \qquad (4)$$

For the special case when there is no reaeration ($K_2 = 0.0$), which is of interest during the winter ice cover condition, Equation (1) has the following solution:

$$C = C_0 + L_0\left(e^{\frac{-K_1 x}{u}} - 1\right) + \frac{(\Phi_C - \Gamma_C)}{u}\, x \qquad (5)$$

APPLICATION OF THE MODEL

Estimates of the dissolved oxygen and BOD concentrations were made for that portion of the Milner Reach between Snake River Miles 654.0 and

640.0. These estimates were obtained from Equations (3), (4), and (5) using various organic loading levels for the NPDES permits. The effect of these loadings upon water quality was estimated for January with no ice cover, January with complete ice cover, March, August, and October. These months were chosen as critical seasons from the standpoint of river flow and in-stream water quality.

The water quality characteristics, river hydrology, and cross-sectional characteristics for each of the months analyzed are described below.

Water Quality Characteristics

The water quality characteristics for the Snake River at River Mile 654.0 were estimated from the results of surveys made by EPA Region X in 1971, 1972, and 1973. The data from these surveys are stored in the EPA's STORET system. The concentrations of temperature, dissolved oxygen, and BOD used in the analysis are shown in Table 1.

Table 1. Water quality characteristics of the Snake River at River mile 654.0

Month	Temp. (C)	D.O. (mg/1)	B.O.D. (mg/1)
January (no ice cover)	0.0	11.3	1.5
January (100% ice cover)	0.0	11.3	1.5
March	5.0	9.9	1.5
August	22.0	6.4	1.5
October	10.0	10.0	1.5

Water quality for the surface and ground water return flow, assumed to be the same for both sources, is shown in Table 2. Data of this nature for the Milner Reach are limited. It was, therefore, necessary to use estimates made from available data. In this case, water quality studies from the Boise River basin were used as a means for estimating quality of the return flows.

Table 2. Water quality characteristics of surface and groundwater return flow flow in the Milner Reach, as estimated from Boise River data.

Month	Temp. (C)	D.O. (mg/1)	B.O.D. (mg/1)
January (no ice cover)	0.0	8.0	0.0
January (100% ice cover)	0.0	8.0	0.0
March	-	-	-
August	22.0	6.0	1.0
October	10.0	8.0	1.0

Hydrology

Discharge of the Snake River at River Mile 654.0 was varied over a range of flows. The quantity of surface and groundwater return flows was kept constant, as shown in Table 3. These return flows correspond to one-half (50%) of the total return flow in the Milner Reach, as given in the U. S. Bureau of Reclamation's 1971 base flow study. The average monthly and 1-in-10 seven day low flow for the Snake River below Minidoka Dam are also shown in Table 3.

Table 3. Hydrologic characteristics of the Snake River below Minidoka Dam for selected months.

Month	Average Flow (cfs)	1-in-10 Flow (cfs)	Return Flow (cfs/mile)
January	2167	276	4.0
March	3189	488	0.0
August	8750	5528	16.0
October	2488	1593	15.0

River Cross-sectional Characteristics

The Milner Reach below River Mile 654.0 was divided into five segments. River widths and depths were assumed to be constant throughout each of the five segments. River miles included in each segment and corresponding width and depth are given in Table 4.

Table 4. Cross-sectional characteristics of segments in the Milner Reach of the Snake River.

Segment No.	River Mile	Width (feet)	Depth (feet)
1	654-653	1200	4.5
2	653-649	1200	4.8
3	649-645	1200	8.7
4	645-643	1200	4.9
5	643-640	1200	18.0

Rate Constants

The deoxygenation rate, K_1, was assumed to be 0.15 1/days (base e), at 20 C, for the entire reach. This rate was obtained from long term BOD measurements of the J. R. Simplot effluent in March 1972. The rate was adjusted for temperature according to the relationship:

$$K_1 = K_1^{20} \; 1.047^{(T - 20)} \qquad (6)$$

where,

K_1 = the deoxygenation rate at temperature, T, 1/days (base e),

K_1^{20} = the deoxygenation rate at temperature, T = 20 C, 1/days (base e).

The reaeration rate, K_2, was estimated from the method given by O'Connor and Dobbins[1] :

$$K_2^{20} = 12.9 \frac{u^{0.5}}{H^{1.5}} \tag{7}$$

and adjusted for temperature, T, according to:

$$K_2 = K_2^{20} \; 1.024^{(T - 20)} \tag{8}$$

The sediment oxygen demand rates, Γ_C, were obtained from field studies made by Kreizenbeck[2] . Observations were made at four stations, and the results are given in Table 5. It was assumed that the values remained constant throughout each segment. Furthermore, it was assumed that the sediment demand varied with temperature according to the relationship:

$$\Gamma_C = \Gamma_C^{22} \; e^{0.07(T - 22)} \tag{9}$$

Table 5. Observed sediment oxygen demand and corresponding D.O. sink strength in the Milner Reach of the Snake River (after Kreizenbeck[2]).

River Mile	Oxygen Demand ($gm/m^2/day$)	Strength of D.O. Sink (mg/l/sec)
654-653	0.89	7.54x10-6
653-649	1.04	8.21x10-6
649-645	1.85	8.03x10-6
645-643	1.85	14.28x10-6
643-640	5.33	11.22x10-6

Loading Levels

Best practicable control technology (BPT) currently available for the Ore-Ida and J. R. Simplot waste discharges was used as a starting point for the analysis. These loadings, terms of BOD (5 day) are given in Table 6.

Table 6. Organic waste loadings for Ore-Ida and J. R. Simplot in the Milner Reach, as determined by BPT.

Source	BOD (5 day) Load (lbs/day)
Ore-Ida	4100
J. R. Simplot	6300

Field Studies and Model Verification

During October 1974, a comprehensive field study program was conducted in the Milner Reach of the Snake River for the purpose of verifying the mathematical model. In-stream water quality, industrial and municipal discharges, irrigation return flow and river hydrologic characteristics were measured by FPA Region X, EPA'S National Field Investigation Center (Denver), and the State of Idaho's Department of Health and Welfare.

Survey results indicated that irrigation return flow was not significant between Snake River Mile 654.0 and River Mile 640.0. In addition, algal photosynthesis and respiration were found to be important sources and sinks respectively, of dissolved oxygen. Detailed results of this study are reported by Yearsl[1] .

Comparison of predicted and observed dissolved oxygen levels, using data from the October 1974 field study, are shown in Figure 2. Sensitivity of the mathematical model to random errors in sediment oxygen demand, net algal oxygen production, deoygenation rate, reaeration rate and river velocity are reflected by the one standard deviation (σ) band in Figure 2.

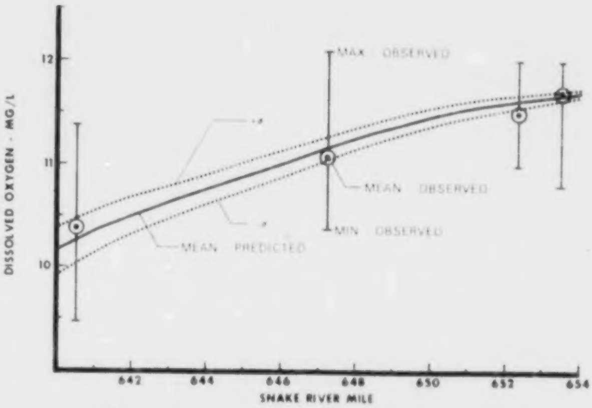
The success of the model in simulating field measurements, coupled with its relative lack of sensitivity to errors in parameter choice, indicated that the model would be useful for the purposes of permit writing. The model, as described previously was applied to the permit writing process. Algal productivity was not included in the permit analysis, since it was felt that this was not a reliable source of oxygen. Simulation results also showed that when algal oxygen production was not included in the model, simulated dissolved oxygen levels were very nearly the same as minimum dissolved oxygen levels measured during the field studies.

PERMIT ANALYSIS

The State of Idaho water quality criterion for dissolved oxygen in the Milner Reach of the Snake River requires that the dissolved oxygen be greater than 6.0 mg/l, or 90% saturation, whichever is greater. For the initial conditions given in Table 1 and loading levels given in Table 6, model simulations indicated that these standards would be violated whenever the flow was less than the monthly average (Table 3). The permits for the two discharges were, therefore, designed such that the treatment levels varied with the river flow. It was assumed that a ten (10) per cent variation in dissolved oxygen at any flow was not significant. The BOD loading from Ore-Ida and J. R. Simplot, only, which caused this much variation was computed, as a function of flow. For those flows resulting in loadings equal to, or greater, than 100 per cent of those values given in Table 6, BPT was acceptable. For river flows resulting in a loading between fifty (50) and 100 per cent of the values in Table 6, advanced waste treatment was required. When the computed loading was less than fifty (50) per cent of the values in Table 6, no discharge to the river was permitted. The resulting flow restrictions, as estimated from the mathematical model, are given in Table 7.

Table 7. Treatment requirements, as a function of flow in the Snake River, for Ore-Ida and J. R. Simplot, in the Milner Reach of the Snake River.

Month	Zero Discharge Below	BPT Above
January (no ice cover)	450 cfs	750 cfs
January (100 % ice cover)	690 cfs	1030 cfs
March	800 cfs	1190 cfs
August	1450 cfs	2600 cfs
October	700 cfs	1300 cfs



PREDICTED AND OBSERVED DISSOLVED OXYGEN IN THE LAKE MILNER REACH OF THE SNAKE RIVER. SURVEY ON 10/22/74 - 10/24/74.

FIGURE 2

REFERENCES

1. O'Connor, D.J., and Dobbins, W.E., "The Mechanism of Reaeration in Natural Streams," ASCE Trans., Vol. 123, 1958, pp. 641-666.

2. Kreizenbeck, R.A., "Milner Reservoir Benthic Oxygen Demand Study," EPA Region X, 1974.

3. Yearsley, J.R., "Evaluation of Lake Milner Water Quality Model," EPA Region X, Working Paper No. EPA-910-8-75-092, 1975, 81 pp.

LOCATION OF MAJOR INDUSTRIAL AND MUNICIPAL DISCHARGES IN THE LAKE MILNER REACH OF THE SNAKE RIVER, IDAHO (OCTOBER 1974)

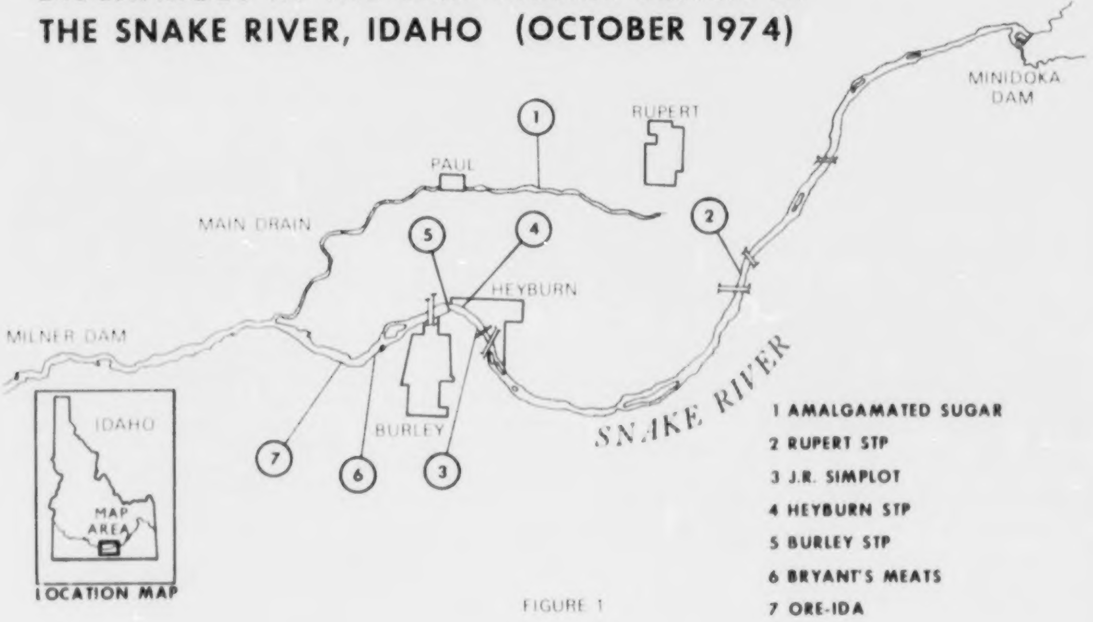

MINIDOKA DAM
RUPERT
PAUL
MAIN DRAIN
HEYBURN
MILNER DAM
BURLEY
SNAKE RIVER
IDAHO
MAP AREA
LOCATION MAP
1
2
3
4
5
6
7
1 AMALGAMATED SUGAR
2 RUPERT STP
3 J.R. SIMPLOT
4 HEYBURN STP
5 BURLEY STP
6 BRYANT'S MEATS
7 ORE-IDA

FIGURE 1

BUOYANT SURFACE JET

Mostafa A. Shirazi
Research Mechanical Engineer
Corvallis Environmental Research Laboratory
U.S. Environmental Protection Agency
Corvallis, Oregon 97330

Lorin R. Davis
Associate Professor
Department of Mechanical Engineering
Oregon State University
Corvallis, Oregon 97330

ABSTRACT

In order to obtain improved prediction of heated plume characteristics from a surface jet, a comprehensive set of field and laboratory data was correlated and used for modification of an existing analysis due to Prych. The correlated data was conveniently subgrouped and used for comparisons with related predictions from the model. This way, all the coefficients such as entrainment, turbulent exchange, drag and shear values were estimated based on the mean of each subgroup of data. Modifications were made to the model to best obtain an overall agreement with the data.

INTRODUCTION

Various mathematical models of heated surface jets are available for the prediction of two and three dimensional plume configurations. Two widely accepted methods are used for solving the equations in these models, namely one based on the integral analysis approach and the other based on the differential numerical analysis methods. The latter approach, while capable of greater generality, is considerably more costly and due to limited funds and resources was excluded from further consideration for this work. However, a certain degree of generality of results is retained by considering only three dimensional plume models herein.

A comprehensive review of thermal plume models is presented in Reference 4. Among the three dimensional surface jet models seriously considered is one by Stolzenbach and Harleman (MIT Model)[3,5], another by Prych[1] and the third model by Stefan, et al.[10] It is outside the scope of this paper to discuss in detail results of all experiments on the three models during our attempt to provide a working program. The MIT model, despite its many fine features, runs into considerable computational difficulties. Prych's model is the result of reasonably successful attempt to remove from MIT's model some of these difficulties. Stefan's model was written for the developed zone alone and thus can't be compared with others directly. Even though it includes wind effects absent in the other two, it ignores the hydrostatic pressure in the longitudinal direction.

In general, the MIT and Prych models yield comparable predictions[1]. The greatest deviation between the predictions of both models and data is in plume width. Both models overestimate the plume width.

An effort is made here to introduce modifications in Prych's model to make it better agree with existing data. These modifications as well as certain other additions, are discussed below.

BUOYANT SPREADING

Stolzenbach and Harleman[3] present an order of magnitude analysis of the momentum equations as applied to the jet. They show that the lateral acceleration of fluid particles within the plume is neglible only when the jet is nonbuoyant. Otherwise, the fluid particles accelerate (spread laterally) due to the influence of two interacting forces, namely, the inertia and buoyant forces. Since the full nonlinear equations of motion describing a buoyant plume are too difficult to solve, the lateral spreading due to buoyant forces in the MIT, and Prych models are calculated independently of spreading due to nonbuoyant forces. The two spreading rates are assumed to make additive contributions, thereby ignoring the nonlinear interaction between the two forces. As a consequence of the assumptions in this linearization their analyses overestimate the plume width when the inertia and buoyant forces are the same order of magnitude (i.e., when the densimetric Froude number is not too large). When the plume inertia forces are dominant such as with strong ambient current or large densimetric Froude numbers, reasonable width predictions can be obtained.

The buoyant spreading function used by Prych is based on the analysis of an immiscible film, such as oil spreading over water that ignores the shear interaction between the fluid systems and the variation in density of the lighter fluid from the edge to the center of the plume. In this analysis, the fluid particles are assumed to move with a velocity equal to the velocity caused by abrupt density waves alone.

In a separate analysis of a buoyant spreading of a pool of warm water, Koh and Fan[6] accounted for the interfacial shear interaction but ignored the actual entrainment of the cool water. They found that near the source the spreading velocity and the fluid velocity used by Prych are the same, i.e.,

$$V_n^2 = c^2 \sim g'H$$

Where H is the local depth of the buoyant pool. However, far away from the source where the shear forces become very important, the fluid front velocity is

$$V_n \sim \frac{g'H}{(\varepsilon/H\rho)} (H/B)$$

Where g'H is proportional to c^2, $(\varepsilon/H\rho)$ is proportional to the shear velocity and H/B is the ratio of the local pool depth to its width. If interpreted in terms of plume spread, this finding implies that spreading velocity is inversely proportional to the local aspect ratio of the plume.

The appearance of the local aspect ratio in the expression for the plume velocity offers an intuitively appealing ground for assuming,

$$V_n^2 \sim (g'H)(H/B)$$

This can also be explained as follows. The lower density of the plume causes it to rise slightly about the free surface of the surrounding water. The height of rise at any point is proportional to the local vertical density difference between the plume and the ambient and the depth of the plume at this point. Since both the density difference and depth of the plume decrease from the center to the edge, this height varies from a maximum at the center to zero at the edge causing the plume to spread in that direction. The spreading rate due to buoyancy is related to the slope of this free surface. Since the height of rise at the center is proportional to $g\Delta\rho_c H/\rho$, the slope of the free surface and thus the spreading rate is a function of $g\Delta\rho_c H/\rho B$.

This slight modification to Prych's analysis was introduced in the model. As a result, a satisfactory fit with data became possible.

DEVELOPMENT LENGTH

Analysis of the jet development zone is complicated because of the need to examine simultaneously the characteristics of a core region as well as a turbulent outer jet region. Stolzenbach and Harleman developed a three dimensional program for this region, but in his modification of the program, Prych adopted a one dimensional approach in which he employed celerity relations for the spreading of the buoyant unmixed core region. He then used the appropriate conservation equations to relate the fluid properties at four jet diameters away from the outlet to the fluid properties at the outlet. The fixed development length of four diameters is based on the assumption of a semicircle with an area $2 B_o H_o$. Prych's development length S_i can be written as

$$\frac{S_i}{H_o} = 6.38A^{1/2}$$

where A is the channel aspect ratio.

Note that the above development length does not change with the initial densimetric Froude number. However, calculations with the MIT model show that the development length does change with initial densimetric Froude number as well as the jet aspect ratio.

Since a better agreement of model predictions with the data is expected if this aspect of the model is also appropriately adjusted, resort was made to laboratory experiments to obtain this information. Experiments were conducted in a still water tank with a heated jet at the EPA Corvallis Environmental Research Laboratory. Several jet aspect ratios and jet densimetric Froude numbers were tested. A hot film anemometer probe was used to traverse the jet development zone laterally at several stations downstream from the outlet. The presence of the core was detected from subdued turbulent temperature fluctuations as well as the temperature level. The coincidence of the increased turbulence fluctuations, the beginning of the temperature drop, and the disappearance of a uniform core at a point downstream of the outlet signaled the end of development zone. The data for this length was correlated to give

$$\frac{S_i}{H_o} = 5.4 \left(\frac{A^2}{F_o}\right)^{1/3}$$

This tentative result is subject to refinement (particularly with respect to the effect of the ambient current) when better experimental investigations currently underway[7] become available. Meanwhile, the use of this correlation was found very helpful to fit the model with available plume data.

FITTING THE MODEL WITH DATA

Reference 2 provides a comprehensive set of data that is a good representation of available experiments both in the field and laboratory. The data provide a wide range of plume conditions with which one can test and accordingly adjust numerous analytical functions of the plume model. The plume model contains a number of free variables such as entrainment coefficient E_o, turbulent exchange coefficients E_h, E_v, drag coefficient C_D and shear coefficient C_F. The magnitudes of these coefficients must be prespecified so that the model produces the best fit with the measured plume characteristics.

In order to accomplish this task, the following procedure is adopted: (a) Data for plume characteristics are subgrouped with a narrow range of certain experimental parameters such as the current ratio, R, the densimetric Froude number, F_o, the jet aspect ratio, A, and the angle of discharge, Θ_o. Each subgroup consists of several experiments and several sources, thus providing considerable degree of realism with respect to possible experimental scatter and variations in experimental parameter scales. The choice of a narrow range in certain experimental parameters was dictated by the desire to obtain as strong a correlation of the data within a given subgroup as possible. (b) For each subgroup, the range and the mean of all experimental parameters are determined. (c) The data are correlated using dimensional analysis and multiple regression methods separately for each subgroup following the procedure outlined in Reference 2. (d) The measured plume characteristics are plotted against dimensionless axial distance using the correlation results. (e) A representative smooth curve is drawn through the mean data and local standard deviations are displayed on both sides of the mean curve to show the scatter. This mean curve is a fair representation of the subgroup, and is represented by the mean parameters obtained in item b above. (f) Finally, the program is used to calculate the plume characteristics in each subgroup for the mean of the experimental parameters R, F, A, and Θ_o. Agreement between the calculated characteristics and the data mean is sought by adjusting one or more of the model coefficients E_o, E_h, E_v, D_D and C_F. This process is repeated for several subgroups, adjusting in each trial one or more coefficients until best fits are obtained to plume characteristics for all subgroups.

It should be pointed out that correlations of each data subgroup are useful mainly for the mean data in that subgroup. They are not universal correlations and cannot be used outside the data range they represent.

The data set most suitable for determining the effects of ambient turbulence on plume behavior is provided by Weil[2,8]. In his experiments, Weil injected heated water at the surface in a turbulent channel from a semi-circular jet at a relatively large densimetric jet Froude number. The discharge was in the direction of the channel current ($\Theta_o = 0$). The jet velocity in all his experiments was held equal to the local channel flow velocity. Since the relative velocity between the plume and ambient water is zero and since buoyancy effects are small due to a high Froude number, dilution is largely due to turbulence effects.

For the conditions of this experiment, the following simplifications can be introduced in the mathematical model: (a) there is no relative velocity between the jet and the ambient water. Therefore the contribution of the terms containing the entrainment coefficient, E_o, can be set equal to zero. (b) For the same reason, contribution of terms containing the shear coefficient, C_F, is also zero. (c) The drag coefficient C_D, is zero because the jet is parallel to the ambient current and the pressure distributions on the left and right hand sides of the plume are identical. (d) For the dimensionless surface heat exchange coefficient, one can choose a typical value of $K = 10^{-5}$ without affecting the calculated plume characteristics greatly one way or another, because we are dealing with small areas and small temperature differences. (e) Since the jet densimetric Froude number is high, the influence of the buoyant forces on the plume spread is not substantial. The plume width grows predominantly due to turbulent entrainment of the ambient water, a mechanism which the model accounts for through E_h and E_v.

Figure 1 is the plot of correlated temperature data showing the local mean and standard deviations. Figure 2 is the replot of the mean temperature data together with several computer calculations based on the model for F = 16, A = 2, Θ_o = 0, and K = 10^{-5}. Calculations are made for several values of E_h and E_v/E_h as well as the free factor of the spreading function, XK1. The plots for the calculated and measured plume width data are shown in Figure 3. The measured width data were closely spaced with excellent correlation. For this reason individual data points were not plotted. Instead, a narrow band showing the spread of all expermental data are presented.

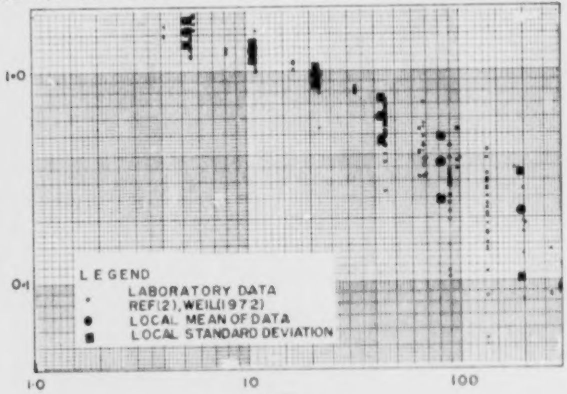


Fig. 1 Correlated Temperature Data for Coflow Discharge, R=1

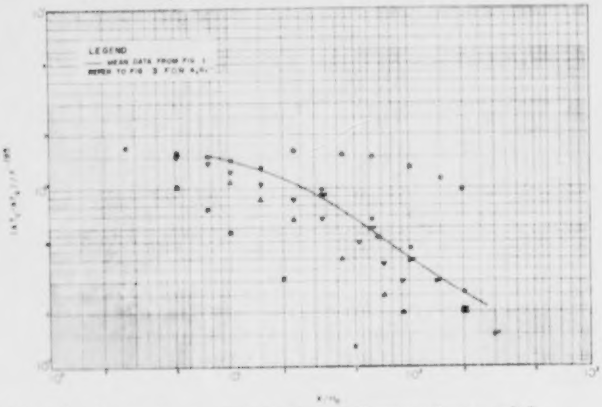


Fig. 2 Comparison of Calculated Temperatures with Measured Plume Temperature Data of Fig. 1

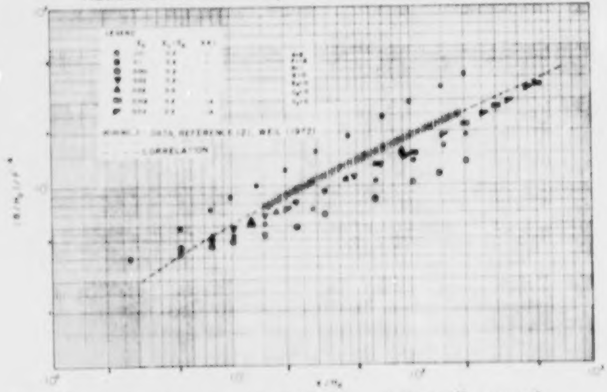


Fig. 3 Comparison of Calculated and Mean Measured Widths for Coflow Discharge, R=1

A visual inspection of Weil's data of Figures 2 and 3 shows that the best fit is obtained with E_h = .02, E_v/E_h = .2 and XK1 = 1.4.

The next group of data consists of information from several sets of laboratory and some field experiments for a surface discharge in zero or negligibly small cross current. The correlation of temperature data are plotted in Figure 4 and the width data in Figure 6.

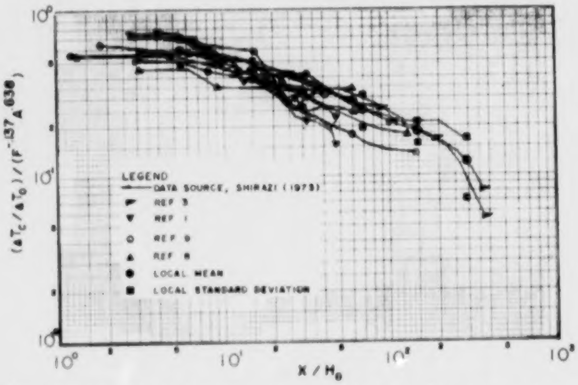


Fig. 4 Correlated Temperature Data for Discharge into Zero or Negligible Ambient Current

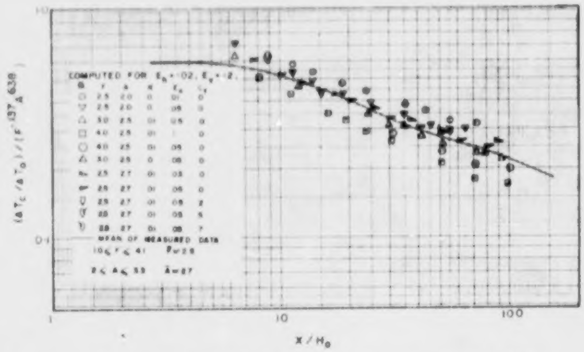


Fig. 5 Comparison of Calculated Temperatures with Measured Plume Temperature Data of Fig. 4

For the conditions of this group, one can assume that the drag coefficient is zero. As a first approximation we also assume that the contribution of the ambient turbulence is accounted for by the previously assigned values of E_h and E_v. As we continue to adjust other coefficients in the model, we may have to reevaluate E_h and E_v.

Figures 5 and 7 show the replots of the mean data and several computer calculations of the model with preassigned values of entrainment and shear coefficients. The best fit of the computer model with the data is obtained with E_o = 0.05. Since the shear coefficient has negligible effect on the result, it will be set equal to zero.

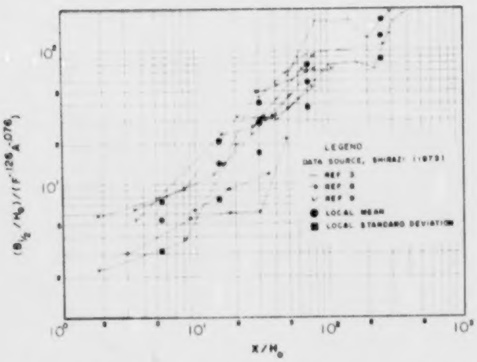


Fig. 6 Correlated Width Data for Discharge into Zero or Negligible Ambient Current

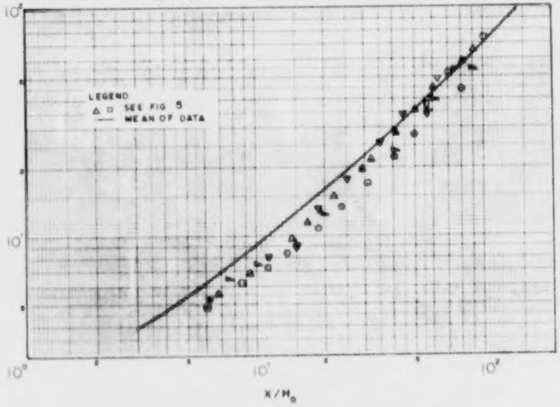


Fig. 7 Comparison of Calculated Widths with Mean Measured Surface Plume Width Data of Fig. 6

For given values of discharge angle, Froude number, aspect ratio, and ambient current, the plume trajectory is mainly influenced by the entrainment of ambient fluid with a minor influence due to pressure drag. Since the entrainment coefficient is prescribed from the above, only the drag coefficient can be used to further adjust the trajectory. Consequently, we need to regroup the trajectory data for a reasonably wide range of all plume parameters mentioned above. Such data are plotted in Figure 8 showing the data sources, the local mean and standard deviations. Figure 9 is a replot of the mean trajectory showing the comparison with computed values. It is found that the best fit is with $C_d = 1.0$.

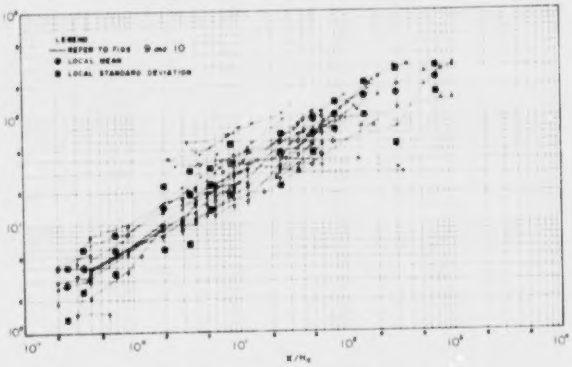


Fig. 8 Correlated Trajectory Data for Discharge into an Ambient Current

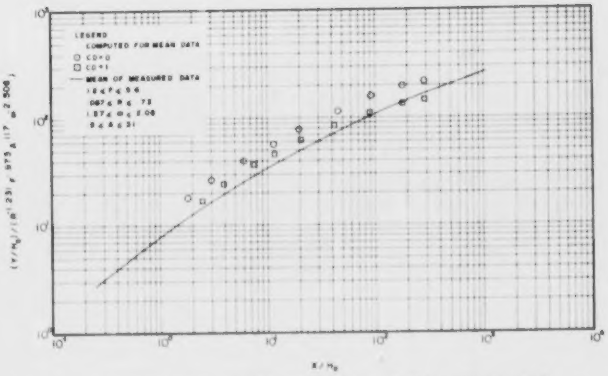


Fig. 9 Comparison of Calculated and Mean Measured Trajectory Data of Fig. 8

In order to complete the adjustment of the model to fit the data, we need to check the model against measured plume width and temperature for a wide range of parameters. If agreement is obtained with such data without the need to readjust the previously specified coefficients E_o, E_b, E_v, C_F and C_D, then the fitting of the model with data is considered complete.

The raw data and calculated values based on previous coefficients are compared in Figure 10 for plume width and Figure 11 for plume temperature. The agreement obtained from the comparison of calculated and measured plume width is excellent and the agreement for plume temperature is reasonably good.

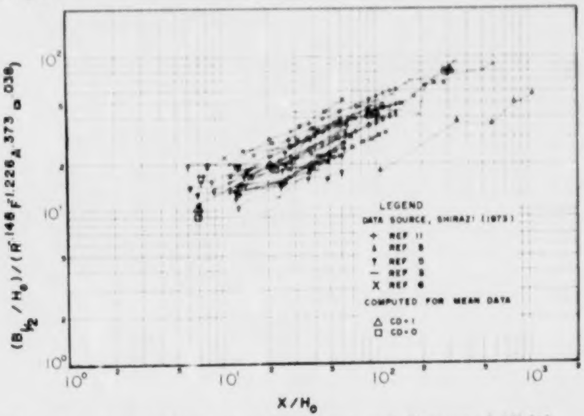


Fig. 10 Comparison of Calculated and Measured Width Data for Discharge into a Cross Current

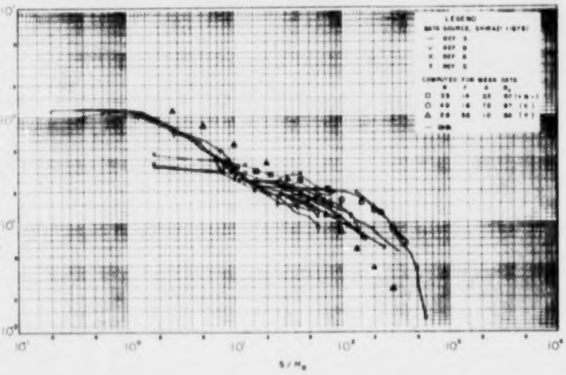


Fig. 11 Comparison of Calculated and Measured Temperature Data for Discharge into a Current

DISCUSSION

A notable degree of data scatter could not be avoided when attempting to correlate information on plume characteristics from several sources. Physical factors not included in the data analysis, but which are believed to have contributed to the data scatter are: a) the lack of a universal simple exponential correlation such as used in this report; b) the influence of diverse turbulence scales, c) the influence of surface heat transfer, d) time dependency and boundary effects, and 3) instrumentation and experimental errors.

The exponential correlations employed are intended for data presentation in a compact form within each data grouping. They are not used to explain the physics of the problem exclusive of the mathematical model. They do, however, provide a statistical presentation of the level of data scatter one can expect when dealing with data from numerous sources.

There are at least two reasons why data from more than one source should be used. These are: (1) there exists no single set of data that covers a sufficiently wide range of parameters relating to initial jet conditions and ambient current; (2) data obtained for a wide range of ambient turbulence levels are reported in the literature. While the ambient turbulence level and turbulence scale affect the plume characteristics, information on these parameters is lacking in nearly all the data reported. It is felt, therefore, that a plume analysis based on several sources carries a greater degree of realism than one based on a single source.

It should be noted that the turbulence exchange coefficient in the model is back-calculated based on the best fit with the data. The coefficient is entered in a form of a turbulent Reynolds number $(H_oU_o/\epsilon)^{-1}$ where ϵ is the turbulent eddy diffusivity and H_o and U_o are the jet depth and velocity respectively. In this manner, even though diffusivities are not directly measured in each experiment the use of the model does provide an indirectly calculated value for the correlation parameter ϵ/H_oU_o that best represents the available data. If in a given application one has a better knowledge of this or any other coefficients entering the model then, of course, those should be used in the model instead.

Calculations based on the foregoing modified surface jet model are presented in great detail in Reference 11. That workbook provides a compilation of numerous nomograms suitable for use in practical prolems. Even though the computer program and sample examples are also given, the use of the workbook directly might be preferrable to the majority of the users.

LIST OF SYMBOLS

B	Local characteristic width of jet = $\sqrt{2}\sigma_n$
B_o	Half width of outlet
$B_{1/2}$	Plume half width = 177 σ_n
C_D	Form drag coefficient
C_F	Interfacial shear drag coefficients
c	Celerity of a density front
D	Local plume depth = $2\sigma_z$
E_h	Dimensionless horizontal eddy diffusion coefficent ϵ_h/U_oH_o
E_o	Entrainment coefficient
EV	Ratio of vertical to horizontal eddy diffusion coefficients E_v/E_h
F_o	Densimetric Froude number at outlet, $U_o/\sqrt{g'H_o}$
g	Acceleration due to gravity
g'	Reduced gravitational acceleration $g\ \Delta\rho/\rho_a$
H	Local characteristic thickness of jet
H_o	Depth of outlet
K	Dimensionless heat transfer coefficient $K_E/\rho c_\rho U_o$
K_E	Atmospheric heat transfer coefficient
s	Curvilinear coordinate along jet centerline
S_i	Distance from outlet to end of initial zone.
ΔT_c	Local excess water surface temperature on centerline
ΔT_o	Difference between outlet and ambient water temperatures
TH	Angle between positive S- and X- directions (Θ)
U_c	Local excess jet velocity on jet centerline
U_o	Discharge velocity from outlet
X	Rectilinear coordinate parallel to ambient current
Y	Rectilinear coordinate, horizontal and perpendicular to X
Z	Coordinate in vertical direction
V	Ambient current velocity
α	Angle used in data analysis of Ref. (2) $\alpha = \pi - \Theta_o$
$\Delta\rho$	Difference between outlets and ambient water densities
E_h, E_V	Ambient turbulent diffusion coefficient for horizontal and vertical directions
Θ_o	Angle between X axis and outlet velocity direction
ν_o	Kinematic viscosity
ρ	Fluid density

SUBSCRIPTS

a	Ambient conditions
c	Centerline value at surface
i	Refers to variables at end of development zone
o	Discharge conditions

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AGROECOSYSTEM - A LABORATORY MODEL ECOSYSTEM TO SIMULATE AGRICULTURAL FIELD CONDITIONS FOR MONITORING PESTICIDES

M. Leroy Beall, Jr, Ralph G. Nash & Philip C. Kearney
USDA,ARS, Agricultural Environmental Quality Institute,
Pesticide Degradation Laboratory,
Beltsville Agricultural Research Center,
Beltsville, Maryland 20705

ABSTRACT

Quantitative measurements of rates and modes of disappearance of pesticides under field conditions are difficult to obtain because environmental parameters cannot be satisfactorily controlled and monitored. A laboratory model agroecosystem was constructed to simulate field conditions which permitted simultaneous measurement of pesticide residues in soil, plants, water and air. The design and construction of five agroecosystems are described in detail. The first phase of research in the agroecosystem was devoted to measuring pesticide residues in air.

Our agroecosystem has a number of advantages, i.e. it is inexpensive, easy to operate, monitor, and sample; versatile in the number of plants and soils that can be studied; adjustable to rainfall and potentially adjustable to wind velocity, light intensity and duration; and conducive to balance studies where pesticide mobility can be compared under similar conditions. It has an advantage over previous systems because the large volume of air exchanged provides cooling, prevents moisture condensation, and permits sufficient air sample volumes for measurement of very low residue concentration. The aerial residues in the exhaust air are trapped on polyurethane foam plugs, which are sampled periodically. Initial results demonstrated that toxaphene and DDT volatilized off of fiber-glass cloths and cotton leaf surfaces, but the rate of volatilization decreased very rapidly with time. Efficiency of trapping by the polyurethane plugs was very high with recoveries >98%.

Our initial objectives are to test the utility of the agroecosystem for comparing the mobility of different classes of pesticides and thereby identifying potential environmental problems. Our long-term objectives are to explore the possibilities of determining bioaccumulation of pesticides in terrestial organisms and interfacing our system with other model ecosystems, particularily the aquatic ecosystem. Our ultimate objective is to devise methods of reducing pesticide mobility.

BACKGROUND

Monitoring the behavior and disappearance of pesticides under field conditions is often difficult for a variety of reasons. Among these is an uneven pesticide distribution on plant or soil surfaces, drift, and volatilization during and after application. Accurate air sampling is difficult because of changes in wind currents.

In an attempt to somewhat control field variability, glass chambers (agroecosystems) were designed and built for monitoring pesticides in the air, soil, water, and on plants. The chambers are large enough to grow many crop species to maturity. Although the concept of model ecosystems for air sampling is not new (Hill et al. 1971), our system was designed to incorporate a new method of sampling air for pesticides. Further, our system is inexpensive compared to elaborate growth chambers. The method consists of drawing air through flexible porous polyurethane foam filters, then extracting the filters with an organic solvent to remove the pesticide for analysis.

In 1970, Bowen reported the absorptive properties of polyurethane foam and used this material to concentrate metallic ions from dilute aqueous solutions. In 1971, Gesser et al. successfully used polyurethane foam to absorb polychlorinated biphenyls (PCB) from water and mentioned that the foam was not specific for PCB, but could absorb organochlorinated pesticides as well. In 1974, Bidleman and Olney found the foam to be highly efficient in trapping PCB from air. We were introduced to the possible use of polyurethane foam for trapping pesticides in air by Taylor, Glotfelty and Turner (1975).

MODEL AGROECOSYSTEM DESCRIPTION

Chamber Construction

Five retangular chambers were constructed (Renwar Scientific Co., Gaithersburg, Md. 20760) and placed in the greenhouse (Fig. 1 and 2). The chambers were constructed from 3/8" (1-cm) plate glass and held together with clear silicone aquarium cement. All sides, top, and bottom were made of glass to assure a minimum of pesticide adsorption and ease of cleaning between experiments. Inside dimensions are 150 cm long, 115 cm high and 50 cm wide. After allowing for a 15-cm soil layer, the remaining volume is 0.75 m^3. To add rigidity and to protect the bottom of the chamber, each chamber was assembled directly and remained permanently in a 3/4" (1.9-cm) plywood tray lined with 1/4" (0.6 cm)-thick felt padding to absorb shock. Walls of the tray are 15 cm high. The chambers were set at a 1% slope back to front.

For servicing, one side of each chamber is equipped with two sliding access panels (72.4 cm high) which ride in felt-lined aluminum channels. Each panel contains two 2.5-cm finger holes for sliding or lifting. When closed, the panels butt against each other, cushioned and sealed by a strip of polyurethane foam weather stripping attached to the end of one panel.

Centered in the front-end of each chamber are two 2.5-cm holes; 5 and 15 cm from the bottom. The lower hole is used to siphon off soil-leachate water and the upper hole is used to collect run-off water. Both ends of each chamber contain 12 5-cm holes for air intake and exhaust. They are centered 20 cm apart vertically and 16.7 cm horizontally, beginning 35 cm from the bottom of the chamber.

Sprinkler Construction

To simulate rain, each chamber is equipped with a

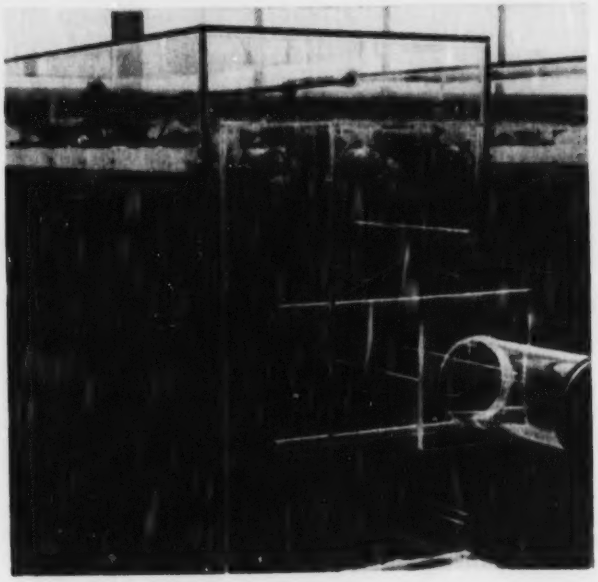

Fig. 1 - Front angle closeup of a model agroecosystem. Note the 12 polyurethane foam plugs in the glass thimbles protruding into the manifold box.

sprinkler system, centered and running the length of the chamber 2 1/2" (6 cm) from the top (Figs. 1, 2, and 3). Each system was fashioned from standard 1/8" brass pipe (ca. 0.6 cm i.d.), threaded fittings, and four spray nozzles spaced 37.5 cm apart. The nozzles (Model 1/8TTGO.3 from Spraying Systems Co., Wheaton, Ill.) each deliver 0.042 gal (159 ml) of water per min at 20 p.s.i. and give a solid cone spray pattern. When "rain" is desired, tap water is supplied to a sprinkler system through a small rubber hose fitted with a quick release coupler. Water supply is controlled by an adjustable pressure regulator and timeclock-controlled solenoid valve. At 20 p.s.i., 1" (2.5 cm) of "rain" is delivered in ca 29 min.

Manifold Construction

An equal amount of suction to each of the 12 exhaust holes is provided by a rectangular manifold box (Fig.1) constructed from 1/4" (6.4 mm) clear acrylic plastic sheet and reinforced inside with six pieces of extruded acrylic tubing 3/4" (19 mm) o.d., 1/2" (12.7 mm) i.d. One end of the manifold contains 12 2 1/4" (5.7-cm) diameter holes to line-up with the 12 exhaust holes in the front of the agroecosystem chamber. Centered on the other end of the manifold is a 5" (12.7-cm) exhaust hole into which was cemented a piece of 12" (30.5-cm) acrylic tubing, 4 1/2" (11.4 cm) i.d. which extends from the manifold box and is reinforced with a 5/8" (1.6-cm) thick x 7" (17.8-cm) square acrylic collar cemented to both the manifold box and the exhaust tube. A 1/2" (1.3-cm) hole, 1 7/8" (4.8 cm) from the blower end, allows entrance for a hot-wire anemometer probe for measuring air speed in the tube. A 1" (2.5 cm) hole is located on one side of each manifold for a manometer connection.

Final connection of the manifold exhaust tube to a suction fan was made with a 9" (22.8-cm) length of 5" (12.7 cm) i.d. flexible-spring-steel-reinforced nylon and vinyl covered hose. This provides an overall distance of 50 cm between the manifold and suction fans.

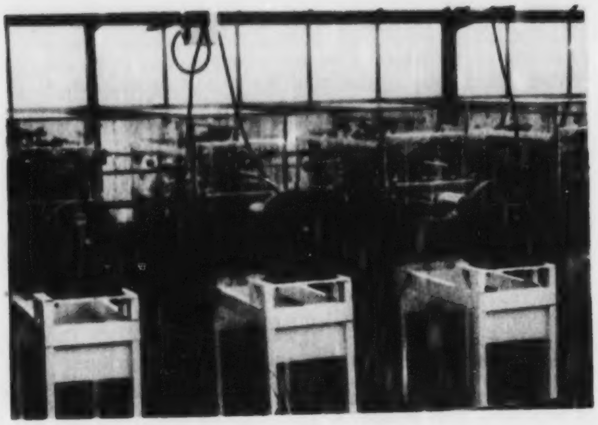

Fig. 2 - Overall view and spatial arrangement in the greenhouse.

Wooden benches support the suction fans and manifold boxes. Latex caulking provides an air-tight seal between the manifold box and agroecosystem chamber.

Air System

Air is pulled through the chamber using a 115 V, 1/3 HP high-pressure direct-drive blower (suction fan) for each chamber. These suction fans provide ca 3 m^3/min air at ca 13-cm water pressure under our conditions. The high-pressure suction fans were necessary to pull air through filters that were positioned in each of the 12 air-exhaust holes of the chamber.

Air movement through a chamber, provided by suction fans, serves three purposes; 1) to collect volatilized pesticides, 2) to provide cooling, and 3) to prevent moisture condensation inside the chamber. Air volumes are calculated by measuring air velocity with a hot-wire anemometer in the tubing which separates the suction fan and manifold box. A mean velocity for each set of 12 plugs is determined by taking 11 measurements (10 equal annular areas and a central circle) at the intersections of a diameter and the set of circles which bisect the annuli and the central circle. Measurements are taken on each side of the cross section at $\sqrt{(2n-1)/10}$ (n=1,2,3 to 10/2) of the tube radius from the center (Perry et al., 1963). In our case, we could only obtain 9 velocity measurements because the physical size of the anemometer prevented measuring of the outer cross-sectional areas. Therefore, the lowest measurement obtained on each side was doubled to approximate measurements 10 and 11. The outer velocity measurements were very low compared to the central circle and the adjacent cross-sectional areas. Typical measurements ranged from 600 to 2000 ft/min (183 to 610 m/min), with the two outer measurements slightly higher than their adjacent inner measurement. The unorthodox velocities near the edge apparently results from turbulance in the short 50-cm length of the tube plus flexible hose between the manifold and suction fan.

Although there was some variation among chambers and among sets of plugs in a given chamber, airflow averaged 2.9 ± 0.3 m^3/min (mean of five chambers and standard deviation). This flow rate translates to an average air speed of 0.22 mph (0.35 km/hr) through the chambers. Our system, therefore simulates calm wind conditions.

Trapping Filters

Pesticide trapping filters were made by cutting 2"

(5-cm) circular plugs from 2" (5-cm) thick polyurethane foam. Cutting was done with a twisting motion of a length of brass pipe sharpened on one end like a cork borer. The foam used was a dark gray, ester base, open cell type with a density of 2 lb ± 10% per ft (ca. 0.032 g/cc) manufactured by the William T. Burnette Co. of Baltimore, Md. Prior to use, the plugs were extracted for 12 hr with hexane:acetone (1:1 v/v) in a Model 11EX/H1 Jobling extractor rigged for Soxhlet extraction. Approximately 46 plugs can be extracted at one time if carefully stacked in the extractor. After extraction, the plugs were squeezed fairly dry and stored in a large rectangular chromatography jar. The remaining solvent is allowed to evaporate before use.

Plugs are held in place (in each of the 12 exhaust holes of an agroecosystem chamber) by thimbles (Fig. 1) fashioned from 45 mm i.d. borosilicate glass tube with 2-mm walls (Renwar Scientific Co.). Total length of the thimble is 68 mm. The intake end of the thimble is expanded to 46 mm i.d. for 30 mm of its length to allow easier insertion of a plug. The rim of the intake-end has a 3-mm rounded lip to retain a rubber O-ring for sealing and to prevent the thimble from going all the way through an exhaust hole. The exhaust end of the thimble contains a glass rod grill to retain the foam plug. The thimbles are installed from inside the agroecosystem chamber and protrude out into the manifold box.

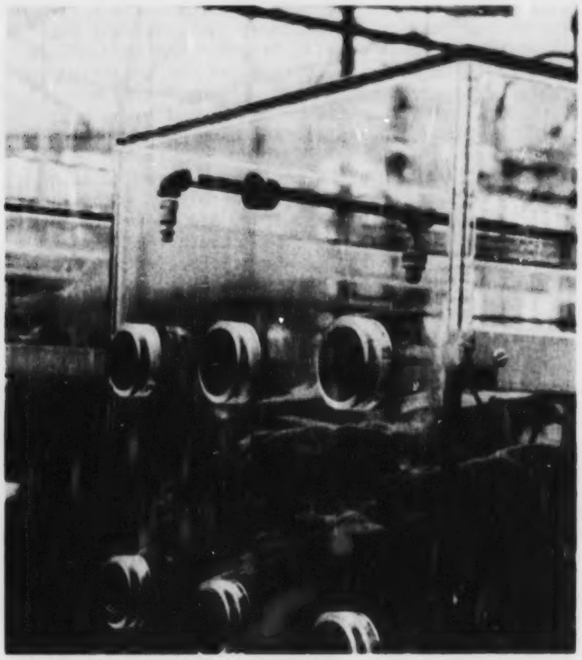

Fig. 3 - Rear angle closeup showing some of the air intake filters and part of the sprinkler system.

Each of the 12 air intake holes on the back of the agroecosystem chamber is fitted with a 2 5/8" (6.7-cm) diameter disk of 1/8" (0.3 cm) thick polyurethane foam air filter to prevent the entrance of insects and dust (Fig. 3). Filter holders were fashioned from clear acrylic tubing. The holder body consists of a 1 7/16" (3.7-cm) length of tube 2" (5 cm) o.d., 1 3/4" (4.5 cm) i.d. with a 3/8" (0.95-cm)-wide ring collar [made from 2 1/2" (6.4 cm) o.d., 2" (5.0 cm) i.d. tube] concentrically positioned and cemented 9/16" (1.4 cm) from one end. The collar limits the distance that the holder can enter the air intake hole. The filter disk is installed by placing it over the outside end of the holder body then pressing a removable ring (same size as the ring collar above) over the disk and holder body. This mechanism provides a quick and simple method for changing the filter disks. Each filter holder is removable but held firmly in its hole in the agroecosystem chamber when pressed through a 2" (5 cm) i.d. rubber O-ring which is cemented around the periphery of the chamber hole. These filters result in slight (0.2 to 0.5 cm water) negative pressure inside the chambers.

Temperature and Lighting

The chambers are subjected to normal greenhouse temperature fluctuations, however, air flow through the systems prevents excessive heat buildup and moisture condensation. On hot sunny days, chamber temperatures may occasionally reach 3°C above ambient greenhouse temperatures. Some moisture condensation was observed on very cool but bright days after the plants filled the chambers.

Recently, a 180 W low pressure sodium vapor light was installed (not shown in Figs.) 5 cm above each of the agroecosystem chambers. The 42" (107 cm)-long tubular lights (from Norelco-North American Phillips Lighting Corp., Highstown, N. J.) are time-clock controlled and can be used to supplement and/or extend daylight periods.

PRELIMINARY TESTS WITH FOAM PLUGS

Extraction Efficiency

Since DDT (1,1,1-trichloro-2,2-bis[*p*-chlorophenyl]-ethane) and toxaphene (chlorinated camphene,67-69% chlorine) were selected to be used in our first agroecosystem experiment, it was necessary to develop a method of extracting these pesticides from the plugs. A group of randomly selected plugs (pre-extracted with hexane:acetone[1:1 v/v]) were treated with ^{14}C-labeled DDT or toxaphene. Treatment consisted of making five 100 μl injections of a benzene solution randomly into each plug. Each plug received a total of 141μg of DDT or 675 μg of toxaphene. Solvent was allowed to evaporate prior to extraction trials. Soxhlet extraction with 150 ml of petroleum ether (30-60°C b.p.) proved to be quite effective. Scintillation counting of aliquots of the concentrated extracts showed that quantitative recovery (based on four replications) of both DDT and toxaphene was obtained in four hours (one plug/Soxhlet). Even with two plugs/Soxhlet, 97.2% of the DDT and 96.8% of the toxaphene was recovered in only two hours.

Pesticide Trapping Efficiency

To test the pesticide trapping efficiency of the foam plugs under conditions similar to the agroecosystems, a plug testing system was built. The system consists of a manifold box connected to a high-pressure suction fan and a set of 12 special plug-holding thimbles. The manifold box and suction fan are essentially identical to those used with agroecosystems, except that the box lays horizontally with the exhaust tube in one end and the 12 intake holes facing upward. The glass test thimbles were made identical to those used in the agroecosystems except that a 5-cm-long widened (5.9 cm i.d. 6.4 cm o.d.) extension tube was added at their rims. The thimbles fit down into the 5-cm diameter holes in the manifold box with the extension tube remaining outside. A rubber O-ring around the thimble (just below the widened extension tube) provides a seal. Polyurethane foam plugs are placed down into the thimbles, then a 10-cm-square piece of loosely woven fiberglass cloth is placed over the end of the thimble extension. The cloth is held in place by pressing a snug fitting plastic ring around the cloth and the rim of the extension. The cloth provides a surface on which a pesticide can be applied. Pesticide molecules volatilizing from the cloth are trapped by the plug as air flows through the testing system. With the suction-fan running, organic solvents evaporate quickly from the cloth, thus, repeated applications of ca. 100 µl of pesticide solution can be made if necessary. Suction created by the fan assures that the volatilizing pesticide is drawn toward the plug.

At the end of a run, the cloths and plugs are removed from their thimbles and analyzed for pesticide content. Pesticide trapping efficiency is determined by summing the amounts in the plugs and on the cloths. If the total is less than the amount applied, the difference is assumed to be the amount not trapped by the plugs.

DDT and toxaphene were tested on the system at room temperature and were both found to be effectively trapped by the plugs. Hexane solutions of ^{14}C-labeled DDT or toxaphene (500 µg pesticide/thimble) were applied and the suction fans allowed to run continuously for 72 hr. At the end of the run the plugs and fiberglass cloths were Soxhlet extracted for 4 hr with 150 ml petroleum ether. Aliquots of the concentrated extracts were counted by liquid scintillation. Of the amounts originally applied to the cloths, 97.45% of the DDT and 99.02% of the toxaphene were accounted for, based on four replications. Of the DDT applied, 30.42% remained on the cloths, while 67.03% was found in the plugs. Of the toxaphene applied only 8.99% remained on the cloths while 90.03% was found in the plugs. Of the amounts of the pesticides that actually volatilized, the plugs trapped 96.33% of the DDT and 98.92% of the toxaphene. During the 72 hr run, approximately 922 m^3 of air passed through each plug.

Efficiency of trapping by the plugs was further tested by applying toxaphene and DDT to fiber-glass cloths as above and harvesting the plugs at 0.5, 2.5, 24, 72, 144 and 168 hr. Fresh plugs were installed at each time period, but the original treated cloths were reinstalled. The plugs were extracted for 4 hr. After 168 hr 97.24% of the toxaphene could be accounted for and 99.90% of the DDT. The fiber-glass cloths contained 6.13% of the applied toxaphene and 56.78% of the DDT, while the accumulative sets of plugs contained 91.11% of the toxaphene and 43.12% of the DDT. These two experiments demonstrated that the polyurethane plugs were very efficient absorbers of volatilized toxaphene and DDT whether the time period was short (0.5 hr) or long (72 hr).

Test Run

For the first experiment, cotton (*Gossypium hirsutum* L., var. 4-42-77 glanded) was treated weekly for 6 weeks with commercial emulsifiable toxaphene and DDT. DDT was sprayed at the rate of 1.33 kg/ha the first 2-weeks, then 1 kg/ha thereafter. Toxaphene rates were double that of DDT. Two chambers were used for DDT and two for toxaphene, leaving one for a control.

The polyurethane foam plugs were harvested and replaced with clean plugs at 0.5, 2.5, 24, 72 and 144 hr after each application. The plugs were extracted and the extract analyzed by gas-liquid chromatography.

The highest insecticide residue concentration in the air occurred the first 30 min (Table 1), then decreased very rapidly with time. After 6 days, residue concentration was only about 5% of that found initially. Toxaphene was more volatile than DDT. The amount of toxaphene volatilized was consistently more than double that of DDT, though the treatment rate was just twice as much. Repeated insecticide applications had little effect on the magnitude of the values obtained after an additional application. The magnitude of the values appeared to be affected more by ambient temperatures than by repeated applications. Even though there was considerable variation in aerial residue concentrations among treatments, the shapes of the curves were almost identical when aerial concentration was plotted against time. A more detailed presentation of the results is under preparation for a following publication.

Table 1. Toxaphene and DDT volatilization from an agroecosystem[a]

Hours after treatment	Compound			
	Toxaphene	*p,p*-DDE	*o,p*-DDT	*p,p*-DDT
	µg/m^3			
0.5	15.108	0.097	1.033	1.720
2.5	9.046	0.065	0.746	1.292
24	2.414	0.017	0.231	0.445
72	1.425	0.008	0.087	0.175
144	0.815	0.005	0.032	0.112

[a] mean of six weekly treatments

Mention of proprietary products does not imply endorsement or approval by the U.S. Department of Agriculture to the exclusion of other suitable products.

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A CONCEPTUAL MODEL FOR ECOLOGICAL EVALUATION OF POWER PLANT COOLING SYSTEM OPERATION

Marc W. Lorenzen
Senior Research Engineer
Tetra Tech, Inc.
Lafayette, California

Carl W. Chen
Director, Environmental
Systems Engineering
Tetra Tech, Inc.
Lafayette, California

Summary

Mathematical models can be useful tools to systematically analyze the impact and significance of cooling system operation. Such models, to have predictive value, must consider the important physical, chemical, and biological processes associated with the cooling system. The first and perhaps the most important stage of this model conceptualization was to select a suitable physical representation of the system. The selected representation provides realistic approximation of entrainment probability, residence times, and material transport in the aquatic ecosystem, the power plant, and the interface, which includes intake and discharge zones.

For a given location, there are physical and chemical properties and biological components including phytoplankton, zooplankton, benthic animals (eggs and larvae), and fishes (eggs, larvae, young, and adult). Interactions among these components are approximated by kinetic expressions for biological and physical processes with particular emphasis on the effect of temperature. The population dynamics of organisms can be influenced by entrainment and the imposed temperature regime. Both direct and secondary impacts of cooling system operation can thus be calculated for interpretation.

Introduction

Installation and operation of large cooling systems may produce many environmental effects. Planktonic organisms (phytoplankton, zooplankton, fish eggs, fish larvae, and benthic animal larvae) may be entrained and suffer direct biological damage: thermal shock, thermal death, mechanical stress and other disruption. At the point of discharge, more organisms may be subject to plume entrainment, thermal shock and turbulence. Dislocation of organisms between intake and discharge points may also be significant. The heated physical environment in the discharge area may influence the distribution of fishes. It may change the temperature regime influencing rooted aquatic plants, which in turn can produce an impact on animal habitat. Nutrient-rich and oxygen-poor water, which may also be saturated with nitrogen gas, may be heated and transported from bottom to surface water.

The direct damage resulting from plant and plume entrainment can induce further ecological effects. Under certain circumstances the loss of eggs and larvae could mean a reduction in subsequent adult populations. Large losses of phytoplankton and zooplankton could alter the patterns of production and predator prey relationships in the receiving water.

The Water Pollution Control Act Amendments of 1972 (PL 92-500) classify heat as a pollutant and provide for regulation of thermal discharges. However, the Act recognizes that not all discharges are necessarily detrimental and provides a mechanism for exemptions to effluent limitations if it can be shown that no appreciable harm would be inflicted on the balanced indigenous community of the receiving water.

Large expenditures may be required to conduct field and laboratory studies to quantify cooling system effects. The collected data must then be analyzed and interpreted to ascertain if a cooling system operation has or will inflict appreciable harm on the balanced indigenous community of the receiving water. Both the direct effects of entrainment and the subsequent manifestations in the receiving water must be determined as quantitatively as possible. A model which can integrate the chemical, physical, and biological characteristics of a cooling system including the receiving water environment would be a useful tool in providing such an analysis. In addition to providing integration of data, environmental or ecological models can and should influence the design and operation of plants. To provide an overall picture, and more importantly, to predict impacts in quantitative terms, a model must consider the important physical, chemical, and biological processes associated with the cooling system.

The general approach to developing such a model has been first to examine specific problems and develop sub-models. These sub-models are then integrated into larger system models. Sub-models include 1) thermal plume simulations to define the area, volume, and residence time of water at various temperatures with in the plume; 2) receiving water transport models to compute entrainment ratios; 3) temperature dose-biological effect models for passage through the cooling system and 4) water quality-ecological models that simulate water quality behavior and population dynamics of the biota.

Prototype Representation

In order to model a complex ecological system it is necessary to carefully select the methods of idealizing or representing the physical conditions and biological processes occuring withing the system. For evaluation of cooling system effects, a physical and a biological representation are necessary. Appropriate units for quantification of environmental characteristics must be selected so that changes can be evaluated.

Physical

Figure 1 shows a general physical representation of a power plant cooling system. The major components of the physical environment which are important to impact assessment are: the boundaries, intake zone, condensers, discharge conduit, and mixing zones defined by water volumes at various temperatures. Each physical segment represents a point or volume for which physical, chemical, and biological characteristics can be defined.

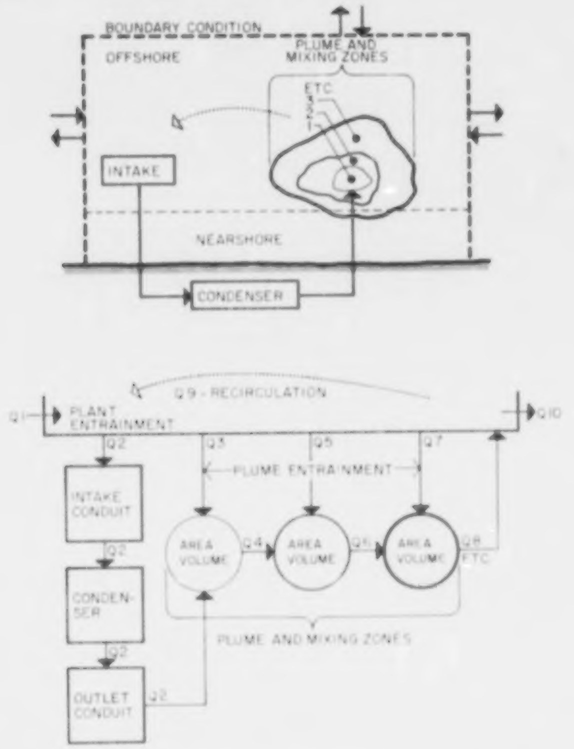

Figure 1. Physical Representation of Power Plant Cooling System

The representation shown in Figure 1 allows for a variable boundary location and recirculation between discharge and intake. The establishment of boundary conditions is extremely important because small-scale models can be completely dominated by the imposed conditions at the boundaries. Ideally, the water and constituents entering the model boundary are not influenced at all by processes occurring within the modeled area. It may be desirable to run several models with different boundaries in order to establish the significance of boundary location. The intake zone must also be carefully defined. A great deal of attention has been given to discharge plumes and circulation. However, it is equally important to know the source of the intake water. The concentration of planktonic oranisms may be very dependent on the origin of cooling water.

The characteristics of the condensers are considered to include temperature changes, pressure gradients, and time of passage. Operational characteristics may be somewhat different than originally designed. For operational plants, measurements should be made to determine actual temperature increases as a function of unit load. Time of passage and pressure changes should also be measured.

The discharge conduit must be considered an integral part of the system. This portion of the cooling system may inflict the greatest damage to plankton because it normally represents the greatest time of exposure to elevated temperatures.

The discharge zone must be considered due to its effects on both plant- and plume-entrained organisms as well as a potential impact on benthos, rooted plants, and fish. The time of exposure to various temperatures within the plume should be known in order to compute thermal doses to entrained organisms.

Biological

Figure 2 shows a biological representation designed for evaluation of cooling system impacts. For each physical segment representing the study area, a system consisting of chemicals, algae, zooplankton, fish, benthos, detritus, and rooted plants can be simulated. The system shown in Figure 2 has only one compartment for each group. However, any number of species or taxonomic groups could be included. The system shown allows for two types of direct impact: plant entrainment and plume entrainment. Mortality is computed directly according to exposure-mortality relationships.

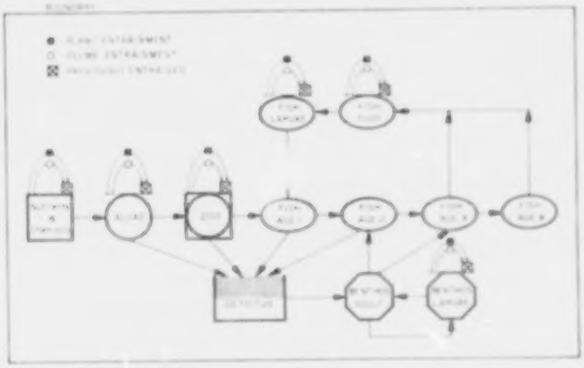

Figure 2. Biological Representation of Power Plant Cooling System

The ecological consequences of the direct impacts are computed indirectly by modeling the larger system. Sub-lethal effects are computed by distinguishing between organisms which have and have not passed through the plant. The pool of organisms which have passed through the plant may have altered survival or reproductive characteristics. "Offspring"of organisms which have been entrained are returned to the "normal" pool.

Mathematical Formulation

The mathematical formulation of the model(s) consists primarily of a set of differential equations describing the rates of change in concentration of each parameter in each compartment modeled.

For example, for constituent i, in compartment k, connected to compartment n:

$$\frac{dC_{i,k}}{dt} = \frac{1}{V_k}\left[\Sigma Q_n C_{i,n} - Q_k C_{i,k} + G - \Sigma L\right]$$

where: Q_n = advective flow from compartment n
Q_k = advective flow from compartment k
$C_{i,k}$ = concentration of constituent i in compartment k
$C_{i,n}$ = concentration of constituent i in compartment n
V_k = volume of compartment k
t = time
G = growth
L = loss

The present conceptualization assumes that advective flows will be input from either hydrodynamic models or an analysis of circulation patterns and plant operation.

The gross growth rate of all organisms is considered to be temperature-dependent. Figure 3 shows a typical relationship between growth rate and temperature. This approach allows an increasing growth rate up to some optimum temperature (range) followed by a declining growth rate at higher temperatures. Gross growth rates are also considered to be "substrate"-dependent as shown in Figure 4. The "substrate" may be nutrients, prey, or light. All growth is considered to be first order with respect to the organism modeled.

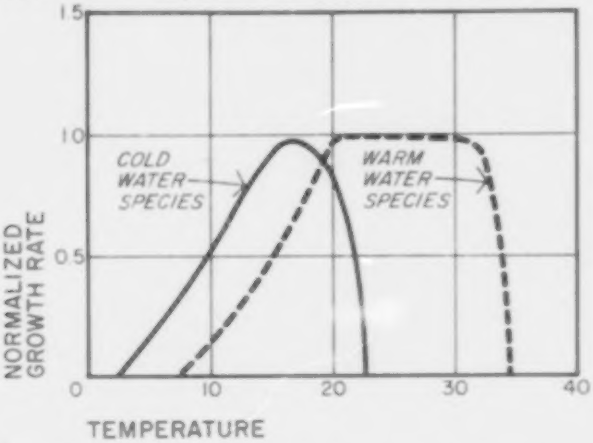

Figure 3. Temperature Modulation of Gross Growth Rates

Loss rates include respiration, sinking, natural mortality, predation, and effects of the plant. Respiration is considered to be a simple first order reaction which increases exponentially with temperature. Sinking rates for phytoplankton are input parameters that can be modified as a result of sudden pressure changes. Predation is considered to be first order with respect both to the predator and the prey. Susceptibility to predation can be modified as a result of thermal or mechanical stress. The direct effects of the plant must be input as specific functions for each group of organisms. For example, plant-induced mortality can be input as a function of temperature, temperature increase, and time of exposure.

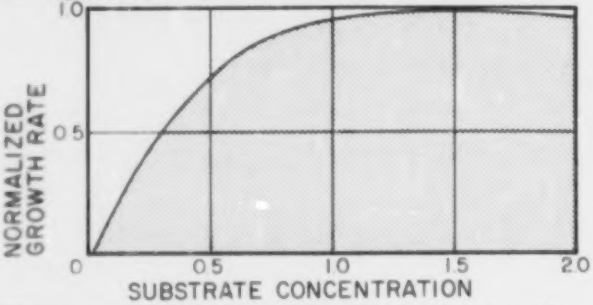

Figure 4. Food Density Modulation of Growth Rate Coefficient

It must be noted that the detailed formulation of growth and loss terms may include the mass concentration of other constituents and coupling effects of the various quality constituents are therefore included in the model. There are as many differential equations as quality constituents and physical compartments modeled. The equations are solved simultaneously to yield the concentrations of each constituent as a function of time. The results can then be assessed to determine environmental impacts of a cooling system.

Modeling Framework

The general framework for model development and application consists of four interacting stages. During stage I, data are compiled for the pertinent biological, physical, and cooling system characteristics. These data relations, temperature-pressure mortality relationships, substrate and temperature growth rate relationships, physical boundaries, bathymetry, circulation patterns, and a definition of conditions to which entrained organisms will be exposed.

During stage II, data are input to a storage and retrieval system. Summaries and statistical analysis can be provide. Regressions and correlations can be determined for possible use in defining relationships needed in the models.

Stage III is the actual model formulation and includes definition of equations and programming modifications necessary for site-specific conditions.

The final stage is the execution of the model. The program can be used for baseline simulations, computation of direct impacts, and ultimate effects in the ecosystem.

Biological Data

The first step in defining the biological system is to determine the major and important components of the ecosystem which may be affected. Importance may be a reflection of food web relationships, aesthetics, economics, or recreational resources. For example, the major ecosystem components of the San Francisco Bay-Delta are the striped bass; king salmon; and the oppossum shrimp, *Neo-*

mysis mercedis. The phytoplankton, zooplankton, and benthos as general groups are important but are less likely to be affected by cooling system operation.

Analysis of the major species or groups must then be conducted to determine life histories and thermal tolerance data. Life histories should be complete enough to determine which life stages are susceptible to adverse effects and when they occur in relation to cooling system operation. Thermal tolerance data should define the effects of short- and long-term exposure to elevated temperatures. For some groups, the effects of exposure to heat are dependent on both temperature increase and time of exposure. An example of this type of relationship is shown in Figure 5. Other organisms, such as Neomysis, experience mortality as a funciton of maximum temperature, as shown in Figure 6.

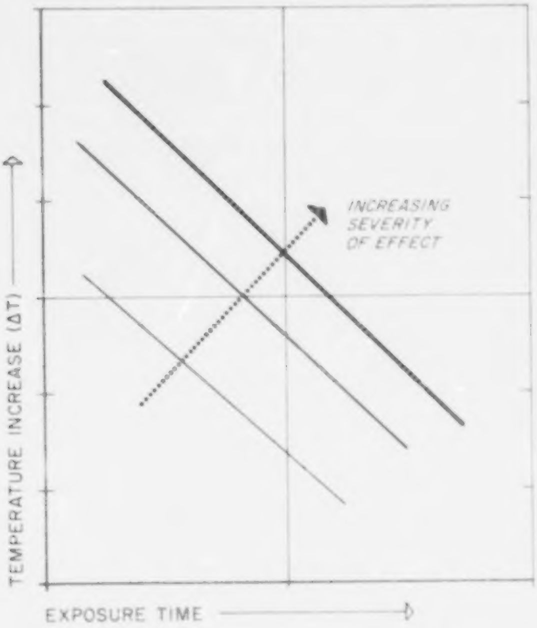

Figure 5. Time-Temperature-Effect Plot

Following identification of susceptible life stages and thermal tolerance data, general relationships between temperature and growth or reproduction rates, mortality rates and spawning activities should be determined. It is important to key these relationships to time as well as temperature in order to integrate the results with plant operational data.

Physical Data

One of the most important and often neglected aspects of cooling system evaluations is analysis of the physical transport of organisms which are subject to entrainment. There are three basic types of physical systems which must be treated differently. Unidirectional river flow is the simplest and normally would require only a hydrologic analysis to relate frequency of river flow to seasons and abundance of organisms of interest. The percent of river flow, or organisms entrained, which is a function of time is then a simple ratio of cooling water flow to river flow. It is necessary to determine the level of lateral mixing and distribution of organisms (side, mid-channel, surface, bottom).

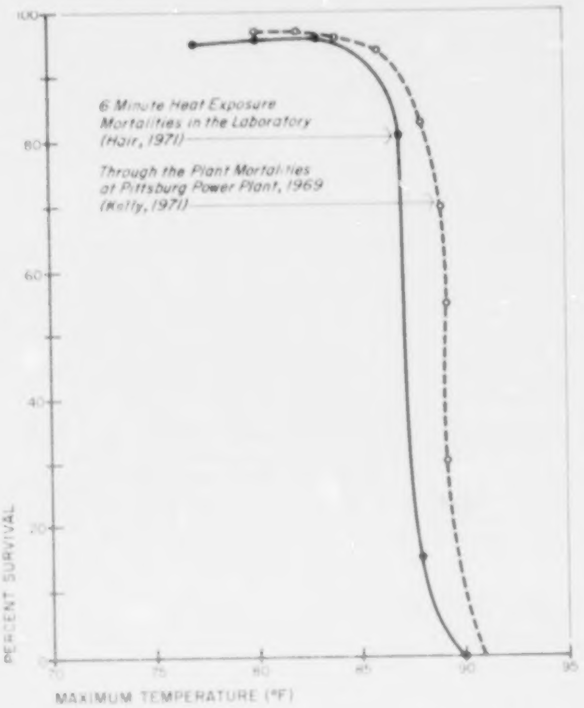

Figure 6. Effects of Elevated Temperature on Neomysis Survival

Tidal estuaries are somewhat more complicated due to the oscillatory nature of the flow. However, an "entrainment ratio" can be calculated with the use of a number of simulation models. Figure 7 shows computed entrainment ratios for a power plant with cooling water flow of 1000 cubic feet per second located mear the confluence of the Sacramento and San Joaquin Rivers on the San Francisco Bay-Delta. The figure shows the fraction of water at each location that would have passed through the power plant if steady-state conditions were reached. The computations were carried out for summer conditions with a net fresh water flow of 4000 cubic feet per second and a typical semi-diurnal tidal cycle.

Open coast locations are the most difficult to quantify due to the uncertain boundary conditions. Coastal currents and circulation patterns can be input as boundary conditions to the study area. However, the definition of the study area is extremely subjective. One approach to this difficulty is to provide an analysis with several different study area boundaries and attempt to assess the effects as a function of study area size. For example, 2% of the zooplankton within three miles of a plant may be killed each day. Whereas only 0.5% may be killed each day within six miles of the plant.

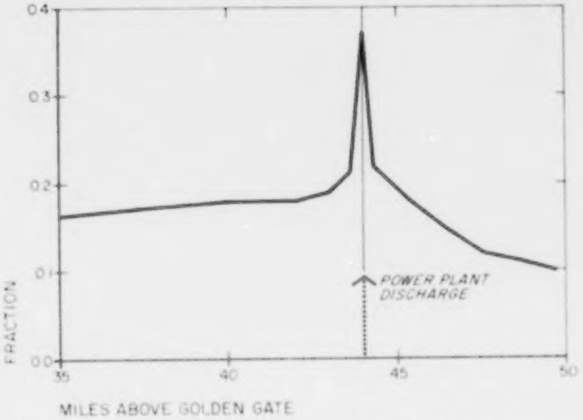

Figure 7. Fraction of Water Which Has Passed Through the Plant Under Steady-State Conditions of 4000 cfs Delta Outflow and 1000 cfs Cooling Water Flow

In general, physical data should include bathymetry, flow regimes, currents, circulation patterns, and entrainment ratios. Thermal plumes should be determined in sufficient detail to describe location, area, volume, residence time, and whether or not the plume affects rooted plants or animals.

Cooling System Data

Cooling system data must be sufficient to evaluate the impacts on both the organisms entrained in the plant and the plume. For power plants it is necessary to define the temperature and time of exposure for plant passage. Most cooling systems consist of a number of units which may have different characteristics. It may be important to obtain operational data describing these conditions through each unit as a function of travel time. Sheer stress, pressure changes, and chemical additions may affect survival of organisms and should be ascertained.

Model Use

Although this model is only in the conceptualization stage, previous work has shown the utility of certain sub-models and confirmed the need for an integrated approach. For example, the design of units 2 and 3 at the San Onofre Nuclear Generating Station calls for extended diffusers on the once-through cooling water system discharge. The design will expose plant-entrained organisms to temperature increases of approximately 20°F for 7 to 12 minutes longer than the existing system for unit 1. The model which has been described would be a valuable tool to analyze the significance of extended exposure to elevated temperatures compared to slightly more rapid dissipation of heat in the discharge plume. The significance of alternative effluent locations could also be analyzed.

In another application of a limited modeling approach, hourly power generation data for each of seven units of a power plant were used to compute temperature increases through the condensers. The temperatures experienced passing through each unit were then related to survival of young striped bass using survival functions reported in the literature.[3,4] The percent of young bass which would be expected to have survived plant passage were averaged on a weekly basis. The results are shown in Figure 8. Based on estimates of striped bass abundance in the intake area, the number of fish passing through the plant were estimated and the cumulative number killed were computed.

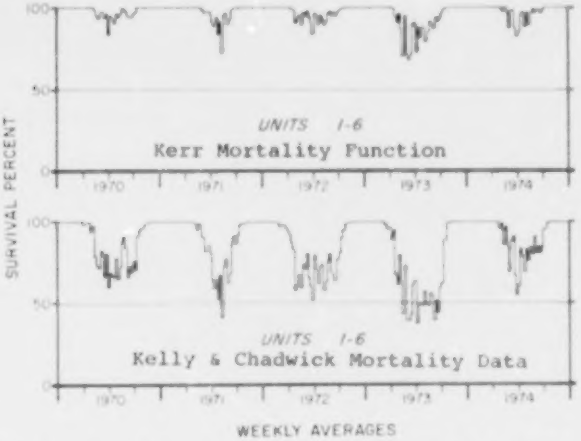

Figure 8. Computed Percent Survival of Young Bass Passing Through a Power Plant Cooling System

Unfortunately, time and funds have not permitted the analysis to go the next step in determining the significance of these computed mortalities to the overall bass population. Furthermore, the computations are based on a number of assumptions (survival data, power generation-temperature increase relationships intake concentrations). However, the approach is quantitative and provides a systematic appraisal of data needs as well as a methodology for evaluation.

Conclusions

Comprehensive models can be used to provide a rational and quantitative interpretation of data as well as guidance in monitoring program design. Modeling results can be used to evaluate the impact of alternative designs. Although direct effects can be computed and verified with field data, consequences often cannot be verified. The most valuable benefit of modeling is therefore, the capability to project ecological consequences resulting from a variety of assumptions and hypotheses.

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REVIEW OF THE STATUS OF MODELING
ENVIRONMENTAL NOISE

William J. Galloway
Bolt Beranek and Newman Inc.
Canoga Park, California

ABSTRACT

Models for predicting the noise produced around airports and highways have been developed over a period of years, have reached a reasonably high degree of accuracy, and are in widespread use. These models provide site-specific information. More recent models have been developed to predict general urban noise and noise produced by construction equipment and other major noise sources. Differentiation is made between models for a specific site, as required in environmental impact reports for specific projects, and models predicting the total population exposed to noise, as used in assessing proposed noise source regulatory actions. The effect of noise source data requirements, sound propagation modeling problems, and operating condition specifications on modeling precision and accuracy are discussed using specific examples relevant to current EPA activities.

BACKGROUND

Acoustical modeling uses both scale model analogs of a real environment and simulation through mathematical models. Physical scale models are used primarily to study sound propagation phenomena in the presence of complicated geometric configurations, e.g., inside a building, between buildings in an urban area, the effect of barriers along a highway. As such, these models consider a restricted geographic area, use artificial sound sources that usually do not scale in magnitude to their real counterparts, and do not generate sound levels representative of a real environment.

Mathematical models of noise environments, on the other hand, are used to predict noise environments at a point, over a local area, or even to estimate national noise exposure. Existing models vary widely in detail, scope, and purpose. The purpose of this paper is to review the general characteristics of simulation models for predicting noise environments and provide a current status report on existing models.

GENERAL CHARACTERISTICS

An acoustical model can vary widely in terms of its sophistication. For example, the noise produced at a point 20 m to the side of a level road by an automobile traveling at a constant speed is a simple algebraic expression involving only a constant with speed and distance as variables. On the other hand, modeling the noise produced in a community from a complex stretch of highway, complete with multiple lanes of traffic moving at different speeds with different vehicle mixes, curving roadways at varying grade levels, including the effect of noise barriers, requires a sophisticated program operating on a high speed scientific computer. Each model, however, has certain attributes in common:

1) Information on the magnitude, frequency distribution of sound level, and time variation of the source must be provided.

2) A propagation model from source to receiver needs to be defined.

3) A measure of noise suitable for use in describing human response is required.

The complexity of the modeling process relates directly to which of these points receives the most emphasis. For example, the designer of a jet transport aircraft attempting to predict whether a new aircraft will comply with FAA noise regulations will put essentially all his sophistication into describing the noise sources in detail so that he can predict the time pattern of sound pressure levels in one-third octave frequency bands at a point on the ground during a flyover of the aircraft. The airport planner, on the other hand, wants to compute the cumulative noise exposure, at points in the entire community surrounding the airport, produced by the total complex of different aircraft and flight paths used at the airport. For this purpose the noise source descriptor is chosen to be as simple as possible, with the emphasis in the model being placed on summing the contributions, at many points in the surrounding area, from the variety of sources involved.

Finally, again using aircraft as an example, it is often of use to have a model in which all the operational factors, propagation characteristics, and exposed population distributions have been aggregated in such a way that changes solely in source strength can be related directly to national impact. Evaluating the impact on the national noise exposure of retrofit noise control measures for the air transport fleet is an application of such a model.

In the following discussion examples of these three levels of modeling will be considered, the "micro," "macro," and "global" approaches. The examples are primarily aircraft and surface transportation noise sources, since, by far, these are the pervasive sources of environmental noise and thus have the most well developed noise models. Models for factories, construction sites, refineries, and other sources of community noise have been developed to a much lower state of sophistication only because of their lesser importance as major noise contributors to the national noise environment.

Before describing environmental noise model building history, it is worth noting that one of the primary psychoacoustical controversies in community noise evaluation, the selection of a community noise descriptor, has been only a minor factor in the physical and mathematical evolution of noise model development. Whether loudness level, perceived noise level, A-weighted sound level, or any other of a myriad of noise descriptors is chosen, the physics of the model building process is basically unchanged. The only circumstance where choice of noise measure has influenced the model development process is in the desire in some models to predict measures of the time distribution function of noise level, for example the median level, denoted L_{50}, or the level exceeded 10 percent of the time, L_{10}. It is usually fairly simple to estimate such measures for a single class of noise sources assumed to produce normal distributions of level with time. Where multiple sources having different time distributions are involved, estimating the combined distribution function is almost hopeless.

Fortunately, the relatively recently evolved international consensus that community response is most directly related to the mean square value of sound pressure, averaged over a specified time period, greatly simplifies the modeling process. With this assumption, the contributions of individual sources to the cumulative noise exposure at a point is a simple mathematical process. A major step forward in developing a unified presentation of model results was the EPA publication of its "Levels" document[1] in which it prescribes that all environmental noise, irrespective of source, should be specified in terms of average (sometimes called equivalent) A-weighted sound level over a specified time interval. This quantity is simply ten times the logarithm of the time integral of A-weighted, squared sound pressure, divided by a specified reference time (one hour, twenty-four hours, etc.) and reference sound pressure. A number of simplified expressions for calculating this measure for typical time distributions of noise signals are provided in Appendix A of Ref. 1.

SURFACE TRANSPORTATION MODELS

Noise from motor vehicles is the most extensive source of noise in most communities[2]. Most early attempts to model noise from traffic have considered the "freely flowing" case of a freeway on flat, open terrain. One of the first models used a Monte Carlo simulation of a Poisson flow of vehicles to predict the noise level distribution at a point as a function of vehicle speed and mean traffic flow volume[3]. Later models generally assumed a uniform distribution of vehicles along a roadway, and for high volumes obtained the same answers as the Monte Carlo simulation[4].

One of the first attempts to simulate a complex flow of traffic, expanding on the Monte Carlo simulation was completed in 1967[5]. Although the simulation was performed with a computer, the model was really not suited for routine analysis of highway problems, in that highway configuration, grade differences, and other real highway configuration effects were not considered. The first design guide provided by the Highway Research Board to account for these factors was completed in 1969[6]. The attempt here was to reduce the simulation results to a series of nomograms suitable for use in hand calculations. The procedure was still cumbersome, and was first programmed for computer use by the Michigan Highway Department. An alternate model, similar in nature, was developed by the Transportation System Center in 1972[7].

An impetus to use these models routinely was provided by the requirement of the Federal Highway Administration[8] that noise predictions for highway planning and improvement projects be performed in all federal-aid highway programs. Meanwhile, with more highway departments using the models a number of noise measurement programs were conducted to determine the accuracy of the models. It was also found that hand implemented versions of the models were not sufficiently detailed to satisfy many highway designers. An improved program incorporating many detailed refinements and reflecting the measurement program results was developed in 1974[9] and is now available in Fortran versions for CDC and IBM computers. Another model developed by the Ontario Ministry of Transportation also appeared in 1975[10].

The present state of highway noise simulation is represented by the HRB, TSC, and Ontario models. Each has detailed differences and varying ease of application, but is capable of predicting environmental noise to accuracies of the order of a few decibels of the real values obtained from validation measurements[11].

AIRCRAFT NOISE MODELS

Simulation of the noise produced by aircraft operations has had a history similar to that of highway noise. Early airport noise models were designed to provide a means for computing the noise produced at a point by a number of different aircraft, generally clustering operations by general aircraft types, e.g., transport aircraft, fighters, propeller-driven, using nomograms and manual computation[12]. Means were provided to develop families of contours of equal noise exposure that could be used to define the total noise environment around an airport if one knew the number and kind of aircraft involved and the flight tracks flown. An improved version was implemented as a Fortran program in [14], but still did not provide for detailed consideration of individual aircraft performance, and required summation of individual contours by a hand drafting procedure.

Implementation of the Environmental Policy Act by the Department of Defense and the Federal Aviation Administration gave impetus to the development of substantially more refined airport noise models in the past few years. Using somewhat different mathematical approaches to achieve the same goals, two major computer programs have been developed by FAA and the Air Force[15,16]. These programs now allow input of the detailed performance characteristics of individual aircraft, variation in power management schedules during a flight operation, dispersion in flight paths, variations in atmospheric conditions, and a host of other improvements. Output is now available in completed contour form through the use of highly sophisticated plotting routines.

The accuracy of airport noise model predictions is very much a function of the accuracy of the input operational data. Noise source characteristics of aircraft are quite well known, but the ability to describe flight paths accurately is difficult. Further, the accuracy of noise prediction decreases as the distance from the aircraft increases. The daily average noise level of a complex of operations can be predicted to within one to three decibels for distances of up to 10,000 feet from a flight path. At farther distances the accuracy decreases due to variation in both knowledge of where the flight paths really are and variation in sound propagation in a real as compared to ideal atmosphere.

Two additional approaches to aircraft noise modeling are of interest. One very ambitious effort at NASA Langley Research Center is a long term project to permit noise prediction as a function of detailed aircraft design characteristics[17]. This program consists of a series of individual modules related to state-of-the-art prediction of individual noise sources such as jet noise, compressor noise, etc., and an executive program to combine the individual component effects into a composite of the noise produced by the whole aircraft. The goal here is to upgrade individual models as the knowledge of detailed source predictions improves. This is in contrast to the usual airport noise models that treat the overall noise of an aircraft directly.

The second approach is a "global" model of airport noise that predicts total population exposed to a specified noise value in terms solely of current aircraft fleet noise characteristics and numbers of operations--either for a single airport or for all air carrier airports[18]. Use of this model allows a simple calculation of changes in population affected by a source noise change, or change in numbers of operations. This model is currently used by the Civil Aeronautics Board as a screening tool in airport/route changes to determine whether a change is minor or major, and thus requiring more detailed analysis[19].

URBAN NOISE MODELS

No suitable models exist for predicting general urban noise from a collection of discrete sources. A first cut estimate, based on a statistical sample of urban noise, allows a general space average noise exposure estimate to be made on the basis of population density alone[20]. For any specific location the level may vary as much as ± 8 decibels from this average, depending upon local street structure and traffic volumes. Development of a general purpose urban noise model that accurately accounts for discrete noise sources, local topography, and urban design is the next major challenge in environmental noise model development.

CONCLUSION

Sophisticated models exist for predicting the environmental noise produced by freeway and airport operations. Accuracies of prediction are of the order of a few decibels--comparable to the discriminability of people to assess noise. Generalized urban noise models are not yet available, although some work is in progress.

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COMMUNITY NOISE MODELING

by

Basil Manns
U.S. Environmental Protection Agency
Washington, D.C. 20460

SUMMARY: This paper discusses the use and need for mathematical models for planning, developing, and managing regulatory programs for community noise control. Both sources and propagation noise emission models are essential to determine the beneficial impacts in the community for each new source regulation. Very elementary and statistical models have been used thus far in dealing with the major noise sources. However, as additional noise sources are identified for regulation, the continued use of these elementary models will not show the real benefits of a particular regulation to the community. This paper will focus on the description of models used for urban traffic and freeway noise. Other models used for construction sites or airports will not be discussed in this paper.

NOISE DESCRIPTORS: It must be clearly understood that one role of the Environmental Protection Agency's Office of Noise Abatement and Control (EPA/ONAC) is to reduce and control community noise by developing regulations for noise emission of newly manufactured products, interstate railroad and interstate motor carrier. The EPA/ONAC does not establish ambient standards. It does establish operating standards for interstate rail and motor carriers, and certain newly manufactured products at the time of manufacture. The products identified for regulation are generally based on those that have greatest impact on the community. The Table I shows that urban traffic category is the highest regarding community noise. Home appliance is ranked as high as it is because the impact level goes down to 45 dB.

Community noise requires the inclusion of all the noise in the outdoor acoustical environment. The outdoor community noise environment varies in both magnitude and character at various locations. The community noise environment also varies as time of day. Thus in describing descriptors for community noise it is necessary to determine the time and location of variations in the outdoor noise environment throughout the community in such a manner that the descriptors are relevant to its effects on people located in various land use categories, either indoors or outdoors.

In describing sound and its effects on people the factors to consider are the frequency spectrum, the overall Sound Pressure Level (SPL), and the temporal variations of both spectrum and SPL. To simplify the approach the frequency spectrum has been weighted to the human hearing sensitivity and summed to obtain a single SPL number. This is the A-weighted SPL in decibels, written as dB(A).

Although the A-weighted SPL is weighted with the human hearing sensitivity it is not a perfect method for accounting for a person's perception of the frequency characteristics of a sound. Many other scales have been developed to better quantify loudness and noisiness. The tone corrected perceived noise level better accounts for the human hearing response by differentiating betweeen broadbands and pure tones. Perceived noise levels exceed the A-weighted noise levels typically by 11 to 17 decibels. Because the perceived noise level scale is somewhat more exact than the A-weighted in relating to physical characteristics of a sound to perceived noisiness, particularly for aircraft, it has become a major element in certifying aircraft.

Tone corrected perceived noise level measurement methodologies require complex instrumentation and data analysis to define a sound. Therefore, they have found little application in the measurement of outdoor community noise. The simple A-weighted sound level meter so far appears to serve the purpose adequately. Therefore most analytical and computer models dealing with surface transportation noise impact analysis are based on the A-weighted sound pressure level in decibels.

The temporal variations of the noise level in terms of the dynamic range variations, discrete single event occurences, and the time and length of these occurences can easily be observed on a graphic recorder. In order to cope with these variations statistical descriptors are used. These descriptors give the percentage of total time that the value of the noise is above a given level. Frequently used levels are L10, L50 and L90 corresponding to the sound level that is exceeded 10%, 50% and 90% of the time respectively. Other descriptors used particularly by the EPA/ONAC are Leq and Ldn shown in equations 1 and 2.

$$L_{eq} = 10 \log_{10} \left(\frac{1}{t_2 - t_1} \cdot \int_{t_1}^{t_2} \frac{P^2(t)}{P_0^2} \cdot dt \right) \qquad (1)$$

$$L_{dn} = 10 \log_{10} \frac{1}{24} \left\{ 15 \left(10^{L_d/10} \right) + 9 \left[10^{(L_n+10)/10} \right] \right\} \qquad (2)$$

The Leq is the energy equivalent noise level or the average SPL over a given time period, usually 8 hours or 24 hours. The Ldn is the day-night energy equiva-

Table 1. Summary of Noise Impact in the United States by Category

	Cumulative Number of People Whose Exposure Exceeds Indicated Ldn (Millions)									1975 Noise Impact (Millions of units)	1992 Noise Impact (Millions of units)
	45dB	50dB	55dB	60dB	65dB	70dB	75dB	80dB	85dB		
Urban Traffic	--	--	93.4	59.0	24.3	69.9	1.3	0.1	0	34.6	5.9
Home Appliances	79.7	44.2	17.1	4.4	0.6	0	0	0	0	26.5	3.9
Aircraft Operations	--	--	24.5	16.0	7.5	3.4	1.5	0.2	0	10.2	2.5
Industrial	--	--	--	--	--	16.7	12.2	8.6	3.8	8.2	2.3
Construction	--	--	26.2	8.7	2.4	0.5	0	0	0	6.2	0.5
Freeway Traffic	--	--	13.7	8.1	4.5	2.3	1.0	0.3	0	5.8	1.7
Operators/Passengers	--	--	--	--	--	11.5	11.5	1.6	1.6	5.1	0.7
Rail Line Operations	--	--	2.0	0.9	0.3	0	0	0	0	0.55	0.04
									Total Impact	97.2	17.5

lent noise level where a 10 dB penalty is given to the 9 night hours (10 p.m. to 7 a.m.). The Leq and Ldn levels have been used by the EPA/ONAC to characterize the health and welfare impacts associated with noise. Impulse or single event noise has been shown to cause interference with communication, disruption of sleep, annoyance, and other physiological effects in addition in some cases hearing loss. However, it is not treated separately but averaged into the Leq or Ldn level to describe the health and welfare impacts.

MODEL DESCRIPTORS: The models used to describe the noise levels produced by various vehicles can be used both for highway planning and design projects and for developing strategies and assessing regulatory alternatives of noise emission source regulations. The basis of all models for highway is the description of the noise produced by a single vehicle observed at a fixed point as the vehicle passes along a straight highway. Three basic approaches to the modeling of highway noise have been used, (1) compute the instantaneous noise levels expected for a randomly occurring flow of vehicles along a single lane equivalent roadway, (2) superimpose the individual sources to constitute a flow, assuming vehicles to be uniformly distributed and spaced along a single lane equivalent roadway, and (3) compute the total acoustic power that is distributed along a single lane equivalent roadway. Using these approaches mathematical expressions have been derived that will describe the observed noise level at a given distance as a function of the vehicle speed, the vehicle flow rate, and the vehicle noise reference level. Using propagation theory and empherical correction factors additional parameters such as vehicle noise frequency spectrum, barriers, ground absorption, atmospheric absorption, reflection, and road geometry are incorporated into the model.

A number of equations have been developed to predict the propagated noise level to a given distance. An early equation, equation (3), developed by Johnson and Saunders shows L50 or the median noise level at sufficient distances from the highway and/or at higher traffic densities. The noise source is shown to smear

$$L50=20+10\log V-10\log D+20\log S \qquad (3)$$

out into a line source whose levels decrease by 3 dB per double distance. The variable V is the vehicle per hour, D is the distance from the highway and S is the vehicle speed. Galloway was the first to develop a simulation model that accounts for the statistical

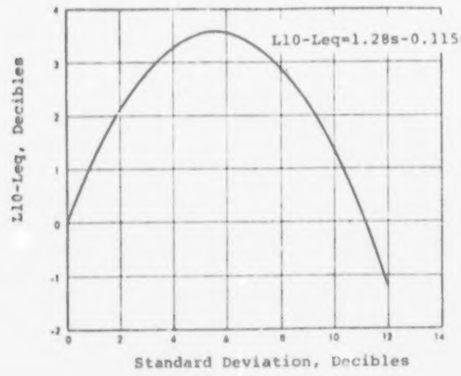

Figure I. Difference between L10 and Leq for a Normal Distribution.

distribution of the noise level as a function of time. The basic equation is shown in equation (4). This

$$L50=29+10\log V-15\log D+30\log S+ \qquad (4)$$
$$10\log(\tanh(1.19\text{x}10^{-3}VD/S))$$

equation is for automobiles, and a similar equation is used for trucks. The variables V, D, and S are the same as above. To convert L50 to L10, equation (5) is

$$L10=10\log\frac{\cosh(1.19\text{x}10^{-3}\rho D)}{\cosh(1.19\text{x}10^{-3}\rho D)-0.95}+L50 \qquad (5)$$

used where ρD is the traffic density. In this simulation empherical expression the traffic represents something between a line source and a point source. Figure I is then used to convert L10 to Leq, since Leq is used by EPA/ONAC as a primary descriptor to assess impact on residential and land use categories. A normal distribution is assumed which is often not a valid assumption for traffic or freeway noise. Another expression developed by the Department of Transportation shown in equation (6), calculates the average intensity for a vehicle group knowing the mean SPL of the vehicle group. The variable r is the reference distance, d the perpendicular distance from

$$I=\sum_{\substack{\text{road}\\ \text{segment}}}\left[\frac{r^2\Delta a}{d}\sum_{\substack{\text{vehicle}\\ \text{group}}}10^{-D/10}10^{L/10}e^{0.5(s/4.35)^2}\right] \qquad (6)$$

roadway, Δa the enclosed angle at the receiver at two ends of the road segment, D the attenuation of sound, L the mean SPL, is the standard deviation of the normal distribution of the reference SPL.
The Leq is the calculated as 10 Log I.

A similar approach developed by Plotkin caluculates the equivalent energy by using equation (7) for each

$$I_j=\frac{d^2}{d_j}\Pi\sum_{k,i}\left[\frac{S_kP_{k,i}I_i}{V_k}\right] \qquad (7)$$

single lane "j" of traffic. I is the vehicle intensity level, P is the fraction of the vehicle that produces a sound level I, S the vehicle passby per unit time, V the vehicle speed, d the passby distance and dj the lane distance. Again the assumption of a line source is used and Leq is found from 10 Log I.

It is really not the purpose of this paper to discuss the details of these simulation expressions or others that have been developed. However, the basic features of these expressions need to be understood to apply mathematical predictive methodologies to assess urban or community noise impact. The important feature in assessing impacts on the community is that a specific site or scenario needs to be defined, including the source since the propagation characteristics of sources do vary.

ASSESSMENT METHODOLOGIES: As part of the requirement of the Noise Control Act of 1972, the EPA identified community noise levels that are "requisite to protect the public health and welfare with an adequate margin of safety." Various land use areas include residential, commercial, industrial, educational, recreational areas, and inside transportation. Generally, Leq levels of 70 decibels are identified to protect against activity interference. Other levels are shown on Table II.

Table II. Noise Levels Protective of Health and Welfare

Human Response	Leq	Ldn
Hearing Loss* (8 hours per day)**	75	--
Hearing Loss* (24 hours per day)	70	--
Outdoor Annoyance	--	55
Indoor Annoyance, Speech Interference	--	45

*Based on exposure over 40 years at ear level.
**As long as the exposure over the remaining 16 hours per day is low enough to result in a negligible contribution to the 24 hour average.

The procedures used to assess impact due to environmental noise follows the same fundamental analysis used for any environmental assessment. First, the initial acoustical environment must be defined. Second, the final acoustic environment must be defined. Third, the relationship between specific acoustic environments and the expected human impact must be analyzed. These three steps are used in planning and developing highway construction projects and also in assessing the impact of planned or developed regulations of specific noise emission sources. When planning and developing a particular road, one uses this assessment approach on a single or group of houses. When assessing the impact of a noise emission source regulation, all houses near the entire national and local highway system are considered.

To simulate various traffic conditions in the United States, the EPA/ONAC has considered both an urban traffic situation and a urban freeway situation. For both scenarios, the models are designed to assess the total United States population affected by particular noise source emission regulations.

URBAN TRAFFIC MODEL: The urban traffic model is a statistical model used for estimating the national urban population benefitted from a regulation. The model uses the following assumptions.

(1) In an urban environment the average speed is 27 mph.

2) The vehicle mixture is 1% heavy trucks, 6% medium trucks, 91.5% automobiles, 0.5% buses and 1.0% motorcycles.

(3) The base line noise levels for each vehicle is heavy truck 85 dBA, medium truck 77 dBA, automobile 65 dBA, buses 79 dBA and motorcycle 83 dBA.

(4) The population density as a function of outdoor noise level is based on empherical data shown on Figure II.

The results shown on Figure II are taken on a sample of 100 sites chosen to represent a wide range of population densities throughout the United States. The sites were chosen away from freeways, construction sites, airports and aircraft noise in order to represent urban traffic noise. The cumulative U.S. population exposed to levels in excess of specific values are shown on Figure III. These data are also taken from the 100 site study and takes into account other noise sources.

The effect of a noise emission regulation on a vehicle category in an urban environment can be assessed by analyzing the change in the equivalent source level produced by changes in the particular noise emission source. Although the equivalent source level Ls, is in dB(A) and the population model is in Ldn, any change in Ls would produce an equal displacement in Ldn. To

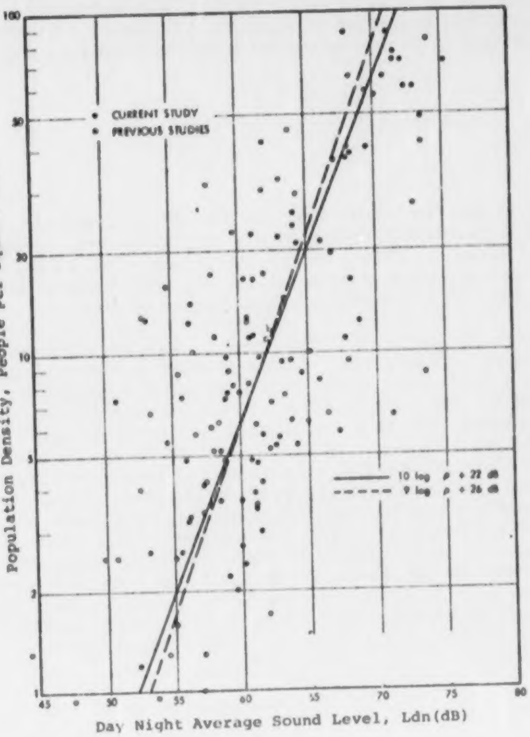

Figure II. Population Density as a function of Day Night Average Sound Level.

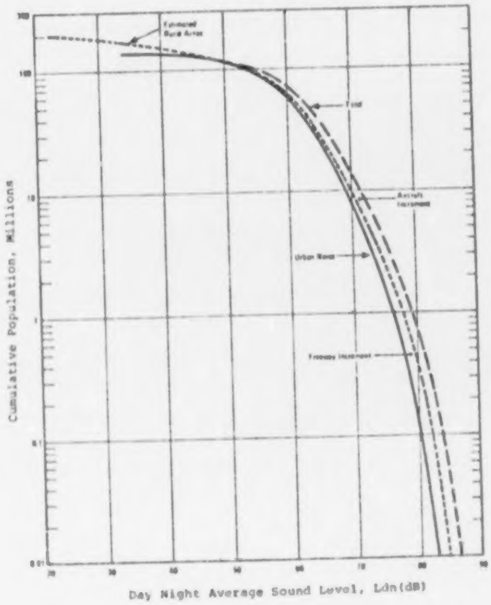

Figure III. Cumulative Population Exposed to Levels in Excess of Day Night Average Sound Levels.

calculate the effect of a noise emission regulation, compute Ls for all noise source categories involved, heavy trucks, medium trucks, automobiles, buses and motorcycles. Knowing the distribution an dthe noise levels of each vehicle, Ls is just the logrithmic summation, expressed in equation (8), where i is the vehicle, Li is the noise level of the i vehicle and

$$L_s = 10\text{Log}\sum_{i=1}^{n} D_i 10^{Li/10} \qquad (8)$$

Di is the fractional distribution of the i vehicle. Ls is calculated before regulatory levels are imposed and after, to determine the before and after conditions for a particular source regulation. The "before" and "after" Ls is equated to equal values of Ldn.

Figure II and III are then used to show relative benefits of a regulation. Figure II shows a lowering of the overall urban noise or din at a given population density. The plot on Figure II will be shifted or displaced left as a result of a source regulation. Additional regulations would also incrementally shift the plot left so that at a given population density the overall urban din can be shown to be less. Figure III, however, shows the cumulative population exposed to levels in excess of specified values. Again since any change in Ls calculated by equation (8) is equal to a change in Ldn, a change in population can be determined that is exposed to levels in excess of the specified values. Thus the number of people actually benefitted by the reduction of the urban noise level is found.

FREEWAY NOISE MODEL: The Freeway Noise Model used by the EPA/ONAC estimates the number of people benefitted or impacted by a particular regulation that live along the miles of urban freeway. As mentioned previously, the analysis to determine the impact due to noise is site specific. For national impact analysis a number of very general assumptions has been used to simulate a site to represent the average urban freeway. The scenario consists of a freeway passing through an urban residential area having the following properties:

(1) Freeway consists of six traffic lanes

(2) Freeway has no grade relative to surrounding property

(3) Population density adjacent to the freeway is 5000 people per square mile

4) Dwellings are single-family, one story high located on one hundred foot lots, two lots deep

(5) Traffic volume is 7200 vehicles per hour with an average speed of 55 miles per hour

(6) Traffic distribution is 10% heavy diesel trucks and 90% automobiles

(7) There are 8000 miles of urban freeway

These assumptions are then used to compute the hourly equivalent levels at various distances from the freeway. The level is computed for both trucks and automobiles and their combinations. The same equation used for the urban traffic model, equation (8), is used for comparing the equivalent source level, usually at 50 feet for a particular combination of sources. The individual source levels used are the levels imposed by the standards being considered. It is assumed that any change in the equivalent source level would produce an equal change in the day night average sound level, Ldn.

The Figure IV represents the noise level adjacent to urban freeways using a 1974 base case of 7200 vehicles per hour, 10% trucks and 90% automobiles, at an average speed of 55 mph. Using equation (8) and calculating the "before" and "after" conditions the change in Ls will produce an equal change of Ldn. Thus an increase in distance from the freeway for the "after" condition is found. The Ldn levels in 5 dB increments from the freeway are computed, and the population in these contours are estimated knowing the population density of 5000 people per square mile and 8000 miles of urban freeway.

It is important to realize that Figure IV illustrates a base case using empherical data representing a situation resembling an average urban freeway. The attenuation is considerably greater than the 3 or 4.5 dB per double distance as described in equations 3 thru 7. The attenuation of 9 dB per double distance is used since this represents the average attenuation of the particular source spectrum expressed in terms of day night average sound level taking into account atmospheric attenuation, ground absorption, building reflection and refraction, and other physical losses. As other sources are analyzed in this model the particular attenuation rate will need to be determined.

PROBLEM AREAS: There are a number of questions that often arise in dealing with the noise descriptors or the models. The descriptors Leq and Ldn have the basic advantage in that they are easy to measure. However, the objection to the use of Leq or Ldn might be that the long term average is not appropriate to describe harmful or annoying effects of short duration, high level noise. This is true where short duration levels may result in permanent hearing damage. However the nature of the decibel is such that an impulse of 110 dB for one second will raise a 24 hour 55 dB average level, to a 24 hour Leq of 62 dB. The average descriptors show an effect to impulse noise and therefore in most cases it is sufficient to use these average descriptors.

Another area which is requiring further study is the use of nationally averaged scenarios to represent environmental impact of various noise emission sources. In using an averaged scenario, the high impact areas are lost in the average. There is a need for a national indicator for assessing the relative impact of various regulations. However, the national indicator would be more meaningful if the average were arrived through a system of scenario sampling. Often more emmision sources are used in certain geographic areas

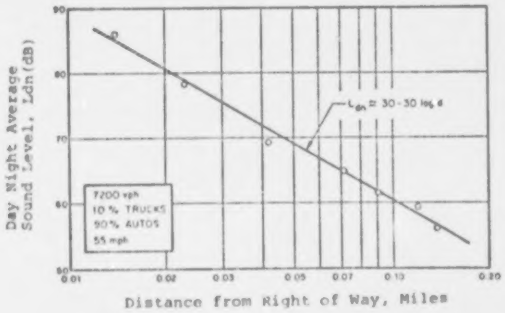

Figure IV. Day Night Average Sound Levels Adjacent to Urban Freeways.

than in others. Many situations exist where communities are severely impacted by highway noise. Other situations exist where expensive noise abatement programs are underway. Obviously all worst case scenarios cannot be found, but a statistical sample of both urban and freeway scenarios can be developed. Techniques are available to accurately predict the levels of exposure in each scenario and determine the number of people impacted.

Currently efforts are underway to look at a number of urban sites and identify characteristic features that could lead to a sampling model. In each scenario site features include acceleration/deceleration areas, lane miles, traffic characteristics (volume, speed, and distribution), topography (vegetation and barrier types), roadway characteristics (configuration and grade), types of housing (single dwelling, or multi-family) and general land use areas such as school, recreation, industrial and commercial areas. These sites could then be used to illustrate a range of scenarios and the impacts and benefits of each regulation could be expressed in terms of specific sites. The next step would be to indicate how these sites represent subgroups within the national population distribution impacted by noise sources.

CONCLUSION: The question that arises when using any model is the accuracy. The data gathered from the 100 sites shown in Figure II indicate that the standard error of estimate of the Log of the population density on Ldn is about 4dB. This is considered analogous to a standard deviation of 4dB. The standard deviation gives the measure of the dispersion of the distribution. However, no data are available as to the variability of traffic mixes used in the Urban Traffic Model. The assumptions used need to be understood in interpreting the results.

Propagation noise model variations are another area where accuracy and understanding of variations are critical. Consider a model which predicts a 70 dB contour at 500 feet from a freeway. If the model over predicted by 5 dB, the 70 dB contour would be 1075 feet from the freeway. An over prediction of 10 dB would move the 70 dB contour out to 2320 feet. Errors of overprediction may cause needless noise abatement programs, either regulations or actual highway barriers, soundproofing buildings or acquisition of public land. Errors of underprediction would cause excessive noise impact on the public.

Finally it should be realized that there is enough known about the characteristics of noise and that technology is available to develop complex models. However, the amount of information required to include all sources of environmental noise, all factors affecting propagation, and the wide range of human responses would be overwhelming. Therefore a number of assumptions has been made to reduce the complexity of the models, primarily because of lack of data. As more data become available the models will include additional parameters to more accurately describe and assess impacts at specific sites and project site impacts to the nation as a whole.

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THE COST OF WATER SUPPLY UTILITY MANAGEMENT

Robert M. Clark
Systems Analyst
Water Supply Research Division
U. S. Environmental Protection Agency
Cincinnati, Ohio 45268

James I. Gillean
President
Act Systems, Inc.
Orlando, Florida

ABSTRACT

Passage of the Safe Drinking Water Act has intensified a growing awareness of problems related to the supply of safe drinking water to the American public. Of major concern is the economic impact which might result from promulgation of regulations under the "Act". In an attempt to understand these impacts, EPA's Water Supply Research Division is conducting a study in which one or more water utilities are being investigated in each of EPA's ten regions. In this paper representative cost data which have been collected from these case studies are presented. These data will be useful in evaluating the economic impact of the Safe Drinking Water Act. They should also lead to a greater understanding of the economic factors which affect the costs of the various components making up a water supply system.

INTRODUCTION

Problems related to water supply have become increasingly important in recent years. In the past, supplying water to the consumer was considered to be a routine matter, and water itself seemed to be available in almost unlimited quantities. But this is no longer the case in most parts of the United States. Perhaps water itself is not a scarce resource, but supplying water of acceptable quality to an increasingly urban population is no longer a simple matter.[2] Spreading urban boundaries force many potential water supply customers to locate farther and farther away from available water sources. Some areas which are inherently water limited have attracted significant population growth, thereby straining the available water resource. A scarcity of the land, labor, and capital resources needed to convey water to places of useful application have contributed to these problems.

Passage of the Safe Drinking Act with its primary and secondary regulations has intensified a growing interest in problems related to water supply and water supply utility management.[5] The primary regulations which are health related and the secondary, non-enforceable, aesthetics related regulations cannot help but have some economic impact. For this reason one of the primary concerns expressed in the Act relates to the magnitude and form of this economic impact upon the American public.

In an attempt to obtain data which can be utilized to assess the Act's economic impact and to understand the factors which influence the cost of water supply the EPA's Water Supply Research Division has been conducting a series of case studies. One or more utilities have been investigated in each of EPA's ten regions. Data from one of these case study areas (Cincinnati Water Works) are presented in this paper. These data are typical of those being collected in the other case studies, and reflect the costs as they affect the functional categories and physical supply problems associated with water supply utility management.

DATA GATHERING PROCEDURES

Water supply systems are generally composed of (1) collection works, (2) purification systems, where needed, and (3) transportation and distribution systems. The collection works either tap a source of water that can satisfy present and reasonable future demand on a continuous basis, or they convert an intermittent source into a continuous supply by storing surplus water for use during periods of low flows. If the water is not of satisfactory quality at the point of collection, it is treated to make it esthetically attractive and palatable.

Water containing iron or manganese is subjected to deferrization or demanganization; corrosive water is stabilized chemically; and excessively hard water is softened. The transportation and distribution works convey the collected and treated water to the community, where it is distributed to the consumers.

Because large operating and capital investments are involved, it is important to be able to compare costs between utilities to understand the components which make up the operation.[3] To make these kinds of comparisons it is necessary to collect the data in a standardized manner. One approach, and the one which will be utilized in this report, is to define the utility's operations in such a manner that they can be categorized into functional areas. Figure 1 illustrates a typical utility in which the operations have been defined as being composed of the functions of acquisition, treatment, and distribution. This is an oversimplified categorization but serves as a useful beginning point. One important area not included is the management function. By collecting data that describe these functional categories it is (in theory) possible to compare the costs of one water supply with those of another. This is the principle that has been used to gather data on the Cincinnati Water Works, although the functional categorizations are much more detailed than presented in the example.

The Cincinnati Water Works operations have been defined as follows: acquisition, purification, transmission and distribution, power and pumping, and support services. These functional categories are common to all water utility operations although the specific costs assigned to each functional category may vary depending on the utility. All of the costs, with the exception of the support services category, are those which make that specific activity operational. Support services includes management, customer services, and all of those costs which do not relate to specific operating activities, for example, laboratory personnel costs are included in the purification activity, but the mangement costs of the purification treatment division are included in the support services category. Maintenance and repair costs are allocated to each category where appropriate.

In addition to the Operating Costs, one must also include Capital Costs in the analysis in order to be complete. For the purposes of this analysis, Capital Costs are defined as the depreciation on the utility's existing plant in service, and the interest on any types of borrowing mechanisms which the utility may use to raise money for capital investment. Depreciation as reported here is based on the actual cost of the facility divided by its useful life, and not on reproduction cost. The data as reported for depreciation, therefore, will reflect lower costs for older utilities. This is true in the case of the Cincinnati Water Works, since most of its facilities were built from 1930 to 1940. In order to understand the magnitude of the bias which such an assumption introduces, an analysis of the replacement cost for the utilities facilities has been made. Using a standardized construction cost index, the original cost of each facility currently in use has been inflated to a 1974 cost base.[4] The analysis is contained in a section which will follow. The interest costs are those which the utility has historically paid for money.

Table 1 summarizes the cost categories utilized in this analysis.

TABLE 1

Operating Costs

- Overhead
- Acquisition
- Purification
- Transmission and Distribution
- Power and Pumping

Capital Costs

- Depreciation
- Interest

All of the cost analysis which will be discussed in this paper is based on revenue-producing water. The unit costs presented will be calculated using the revenue-producing water pumped by each utility during the water year from 1964 through 1973.

SERVICE AREA

The present service area lies almost entirely within Hamilton County with fringe extensions into three adjoinging counties. Although for the most part they are surrounded by the Cincinnati Water Works service area, a number of communities maintain their own systems. Emergency service is provided to most of them, but, as long as their source of supply can be maintained, most of the communities will not change their present status.

The current source of supply is the Ohio River, from which water is pumped to the treatment plant. It has a capacity of 235 million gallons per day (mgd), in 1973 it treated an average of 136 mgd. Water is distributed to the east through a series of pumping stations and tanks. To the north and west, water passes through two gravity tunnels and through two pump stations into a large reservoir and is then repumped into outlying service areas.

COST ANALYSIS

Figure 2 shows the total water pumped by the utility during calendar years 1964 through 1973 as well as metered (revenue-producing) water and water which was accounted for but did not produce revenue. All cost data are based on revenue-producing water, for example, purification costs in dollars per million gallons ($/mil gal) are based on revenue-producing water and not on the total number of gallons of water pumped by the utility. As can be seen from Figure 2, the total water pumped exceeds revenue-producing water by nearly 13,000 million gallons in 1973.

Table 2 contains the total operating cost for each of the previously mentioned categories. The Support Services category includes all of those operating costs that support but are not directly chargeable to the production of water. It includes such items as general administration, accounting and collection, and meter reading. The Purification category includes those costs related to the cost of operating the laboratory, labor involved in the treatment function, chemicals for purifying the water, and maintenance of the treatment plant. Power and Pumping includes those costs related to operating labor, maintenance, and power for pumping water throughout the service area. The Transmission and Distribution category includes the operating labor and maintenance costs associated with supplying water to the consumer.

It can be seen from the table that the Support Services costs have more than doubled between 1964 and 1973. Although all of the other cost categories increased during this period, their rate of increase was less than that of this category. Total operating costs increased by about 65 percent.

Table 2 also contains the total average unit operating costs for each major category based on the number of revenue-producing gallons pumped in a given year. As can be seen, all the cost categories increased by a factor of less than two, and the total operating cost increased by about 40 percent. Each cost category is presented as a percent of total operating cost. It is obvious that Support Services accounted for a significant and increasing portion of the utility's budget, from approximately 26 percent in 1964 to 31.5 percent in 1973. The other cost categories either decreased or remained constant. Depreciation and Interest Expense are defined as the capital expenses for the waterworks system. These capital expenses remained essentially constant but operating expenses increased by approximately 65 percent. As can be seen from Table 2, the percent of expenditures allocated to capital decreased from approximately 27 percent to 22 percent during the period. Operating expenditures are always reported in inflated or current dollars, while capital expenditures are depreciated in historical dollars over a long period of time. The problems related to the depreciation of capital will be discussed later. Since the Support Services category, which is labor intensive, played an increasingly important role in the cost of water supply, labor and manpower costs will be analyzed in the following section.

Labor Cost Analysis

To evaluate the impact of labor costs on operating costs for water supply, it is necessary to examine the payroll of the water utility (Table 3). It can be seen that labor costs accounted for 64 percent of the utility's operating costs in 1964 and for 62 percent in 1973. The average cost per man-hour increased 71 percent, while the number of man-hours/mil gal of metered consumption decreased by 23 percent. The bottom line in the table shows a decreasing capital/labor cost ratio. Although economies of scale were achieved with respect to the number of man-hours used to produce water, the effect on cost was nullified by wage increases. The table, therefore, illustrates the importance of labor in what is typically presumed to be a capital intensive industry.

Depreciation Analysis

As mentioned earlier, capital expenditures comprise a large portion of the cost of water supply. Depreciation reflects historical costs and not the cost of replacing a capital facility based on current costs. Historical costs refer to the original construction cost of a capital facility, while reproduction costs reflect the capital expenditures necessary to build an identical plant today. Historical cost is exact, but reproduction cost is based on the original investment modified by an appropriate index.

The records of the Cincinnati Water Works show the historical value of the plant-in-service to be $111,700,315. The value of pipelines, plant, or equipment previously replaced or fully depreciated is excluded.

Using the historical costs, a reproduction cost was calculated using the ENR Building Cost Index (1913 = 100) for buildings and equipment and the ENR Construction Cost Index (1903 = 100) for pipes and valves. (A skilled labor cost factor is used to compute the Building Cost Index, and a common labor cost factor is used to compute the Construction Cost Index). Having weighted these capital expenditures with the proper indices, a reproduction cost of $458,990,287 was found for the current plant-in-service, which represents a 311 percent increase over the historical value. These capital expenditures do not include the capital investment in a new treatment plant (Great Miami) which is expected to be operational soon. Derivation of a reproduction value facilitates examining the impact of inflation on capital cost and the current worth of capitals contribution to output. The computations discussed in this section are summarized in Table 4.

SYSTEM EVALUATION

Using the cost data for the various functional areas discussed earlier, costs were allocated to specific treatment, transmission, storage, and pumping facilities in the system. A general cost was determined for distribution, interest, and overhead. Using costs based on 1973 $/mil gal and assuming a linear allocation of costs for a given area against capacity required to serve it, the facility costs associated with each service area, such as pumping and storage, were established as shown in parentheses in Figure 3.

The codes in the schematic diagram (Figure 3) can be related to cost values. For example, the acquisition cost for water from the Ohio

River, including depreciation of the facility and operating costs, is $16.70/mil gal. As a unit of water (mil gal) moves through each facility to another service area, the unit cost of moving water through that area is added to the cost of getting water to that area, thereby creating incremental costs. The facility and transmission costs are added to the costs of distribution, interest, and overhead to yield an average unit cost to serve that area. A service zone represents a customer service area and a demand point for water. For purposes of this analysis an attempt was made to discriminate between the water demanded in a given distribution area and the water transmitted through the area into the next service zone.

To illustrate the way in which cost changes from one service area to another, we can examine the B1 and B2 cost areas (Figure 4). The cost per million gallons for area B1 is composed of acquisition cost ($16.70), treatment cost ($60.26), distribution cost ($50.52), interest cost ($17.57), and overhead cost ($85.22). This yields a total cost of $336.86/mil gal. For the B2 area, the pumping and storage costs ($80.45) and the transmission costs ($60.26) must be added to the B1, and this yields a cost of $477.60/mil gal. These values are plotted in Figure 4. The costs in each zone are described by a step function. As water is pumped from the treatment plant through the B1 zone, the average cost per million gallons (using this analysis) remains constant, however, as water is repumped into the B2 zone, the costs take a definable jump to a higher level.

The step function suggests the possibility that as additional service zones are added to the periphery of the utility service area the cost functions will continually increase. It is revealing to compare this costing analysis to the prices actually charged in the utility service area.

PRICING ANALYSIS

Figure 5 is a map of all of the cost zones which make up the Cincinnati Water Works service area. Table 5 contains a comparison between the revenues received from the ten largest users in the service area and the cost of service. It can be seen that many of the major users are not meeting the costs of supplying water to them.

NATIONAL EVALUATION

Cost data for the other water supplies studied have been developed in the same format as presented in this paper. Table 6 contains the costs for these utilities using the cost categorizations discussed. The following approximate breakdown of the percentage of cost which makes up each category is interesting: Acquisition - 15%; Treatment - 12%; Distribution - 29%; Support Services - 24%; and Interest - 20%.

SUMMARY AND CONCLUSIONS

This report documents the application of a functional approach to the analysis of water supply utility management costs. Functionally, these costs have been defined in the following manner: Support Services; Acquisition; Purification; Transmission; and, Power and Pumping. Having defined these costs in a functional manner, they can be reaggregated into capital and operating costs for the various physical components which make up the water delivery system. It is apparent from the first analysis that manpower costs are a significant part of water supply operating costs and that this factor is playing an increasingly important role in the total cost of water as delivered to the consumer. As water is pumped from treatment plant to consumer, costs are added, and they increase with respect to distance from the central supply. By using a specific utility as an example, this kind of analysis can be related to "real world" costs. However, it is obvious that the basic principles discussed apply to all water supplies and that they must be considered in planning and design of water systems. The functional analysis is extremely important for regional considerations. Perhaps the major choice facing most small to medium water supplies will be to join a larger water system or to develop and improve their own water supply systems (4). The approach taken in this analysis should materially assist planners and policy makers in making these types of decisions.

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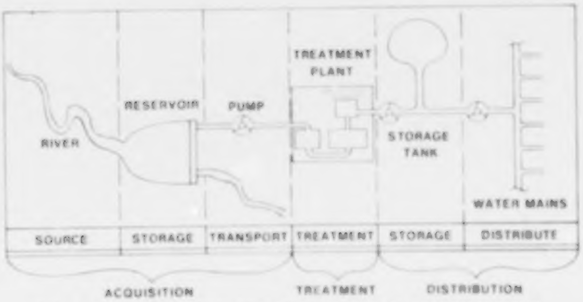
TREATMENT PLANT
RESERVOIR
PUMP
RIVER
STORAGE TANK
WATER MAINS
SOURCE
STORAGE
TRANSPORT
TREATMENT
STORAGE
DISTRIBUTE
ACQUISITION
TREATMENT
DISTRIBUTION

FIG. 1. –SCHEMATIC DIAGRAM OF ACQUISITION, TREATMENT AND DISTRIBUTION FUNCTIONS FOR A TYPICAL WATER SUPPLY SYSTEM

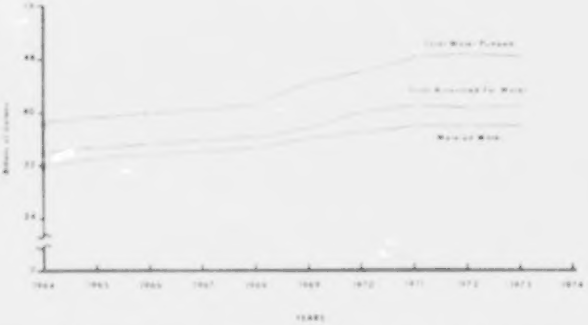

FIGURE 2. Pumped and metered water for Cincinnati Water Works (1964-1973).

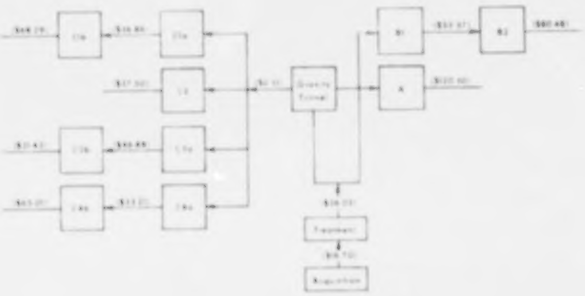
B1
B2
A
($60.48)
Treatment
Acquisition

FIGURE 3. Schematic diagram of facility costs in Cincinnati Water Works system. (To convert $/mil. gal. to $/1000 cum, multiply by 0.26.)

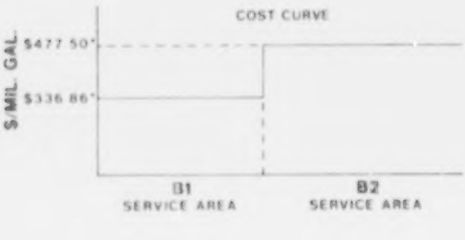

FIGURE 4. Step function cost curve for B1 and B2 service areas. (To convert $/mil. gal. to $/1000 cum, multiply by 0.26.)

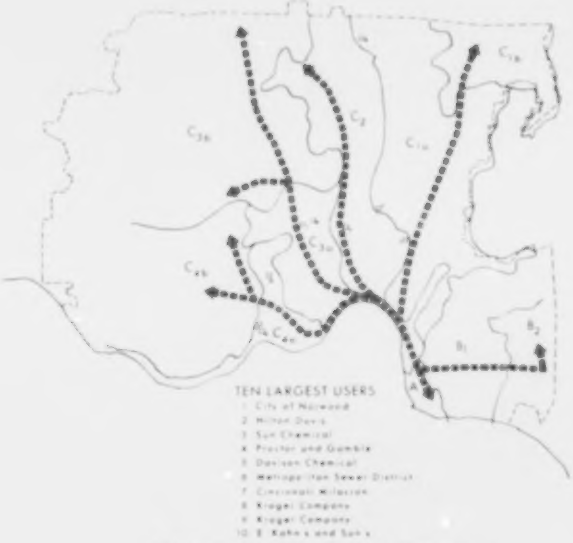
C1a
C1b
C2
C3a
C3b
C4a
C4b
B1
B2
A
TEN LARGEST USERS
1 City of Norwood
2 Hilton Davis
3 Sun Chemical
4 Proctor and Gamble
5 Davison Chemical
6 Metropolitan Sewer District
7 Cincinnati Milacron
8 Kroger Company
9 Kroger Company
10 E. Kahn's and Son's

FIGURE 5. Major facilities in Cincinnati Water Works service area.

TABLE 1. - Operating and Capital Costs*

Item	64	65	66	67	68	69	[illegible]	[illegible]	[illegible]	73
Support Services										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
% of total	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Acquisition										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
% of total	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Purification										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
% of total	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Power and Pumping										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
% of total	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Transmission and Distribution										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
% of total	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Total Operating Costs										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Depreciation										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Interest										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Total Capital Costs										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Total Operating and Capital Costs										
million $	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
$/mil gal	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

*To convert $/mil gal to $/$10^3$ cubic meters, multiply by 0.26

TABLE 2. - Manpower Costs for Cincinnati Water Works

	1964	1965	1966	1967	1968	1969	[illegible]	[illegible]	[illegible]	[illegible]
Total Payroll	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Total Hours on Payroll	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Metered Consumption (MG)*	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Total Payroll ($MG Metered)**	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Total Hours/MG*** Metered Consumption	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Average Cost Per Man Hour	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Capital/Labor Cost Ratio	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

* To convert metered consumption in million gallons to 10^3 cubic meters, multiply by [illegible]

** To convert payroll in dollars/million gallons to dollars/10^3 cubic meters, multiply by 0.26

*** To convert total hours/million gallons to total hours/10^3 cubic meters, multiply by 0.26

TABLE 4

Historical and Reproduction costs of Plant-In-Service for Cincinnati Water Works (Dollars)

Capital Facility	Historical Cost	Reproduction Cost (1973-74 Dollars)
Plant	42,649,160	146,981,272
Pipe	54,848,943	296,771,626
Misc. Plant*	13,202,213	15,237,389
Total	110,700,315	458,990,286

*Capital expenditures which are not specifically identified.

TABLE 5

Actual Charge Versus Cost Comparisons for Ten Major Users In Cincinnati Water Works

User	Revenue ($/MG)	Cost* ($/MG)
Norwood	196.12	272.86
Hilton Davis	166.93 178.47	267.59
Sun Chemical	169.92 175.64	271.56
Procter & Gamble	300.70 321.17	275.76
Davison Chemical	87.06 180.26	277.60
Metropolitan Sewer	175.19 182.44	261.56
Cincinnati Milacron	175.07 187.95	272.90
Kroger Company (Suburb)	113.54 170.28	261.84
Kroger Company (City)	181.80 197.73	264.58
E. Kahn's Sons	182.67 193.17	264.58

*The value for $/MG (dollars per million gallons) can be converted to dollars per 10^3 cubic meters by multiplying by 0.26.

TABLE 6. - Summary of Costs for Utilities Studied (1973-74)

Utility	1973-74 Billed Consumption (bil gal/yr)	Acquisition ($/mil/gal)	Treatment ($/mil/gal)	Distribution ($/mil/gal)	Support Services ($/mil/gal)	Interest ($/mil/gal)	Private Utility Taxes ($/mil/gal)	Total Cost ($/mil/gal)	Dividends ($/mil/gal)
Kansas City, Mo.	26.9	15.28	81.98	138.64	144.52	50.32	-	430.70	-
Dallas, Texas	63.0	25.17	51.70	119.91	83.46	57.71	-	337.95	-
San Diego, Calif.	47.2	279.61	27.47	105.86	95.64	6.73	-	515.31	-
New Haven, Conn.*	17.7	28.97	15.38	107.34	118.19	116.70	196.44	583.02	87.86
Fairfax Co. Virginia	19.2	34.79	61.54	128.33	88.27	208.57	-	521.50	-
Kenton Co. Kentucky	2.2	12.41	102.60	124.41	81.63	73.26	-	394.31	-
Orlando, Fla.	12.5	39.65	25.51	132.82	110.31	85.12	-	393.41	-
Elizabeth Water Co.* New Jersey	38.2	59.52	42.07	111.45	89.80	113.16	96.71	512.71	45.63
Cincinnati, Ohio	38.1	16.70	60.26	127.41	72.60	17.57	-	294.54	-

*Privately Owned

MATHEMATICAL MODELING OF DUAL WATER SUPPLY SYSTEMS

Arun K. Deb
Roy F. Weston, Inc.
West Chester, Pennsylvania

Kenneth J. Ives
University College London
London, England

ABSTRACT

A small percent of total domestic water usage is usually required to be of potable water quality; the rest of domestic need may not warrant excellent quality. Dividing water supply into two portions, potable and nonpotable, a mathematical model of conventional and dual supplies has been developed to evaluate the technical and economical feasibility of dual supplies under various conditions. The sensitivity of the model has been evaluated for various parameters.

INTRODUCTION

Technological advances coupled with increases in population during the past decades have caused the demand for fresh water and the discharges of effluents and wastewater to rivers, lakes and coastal waters to increase. A fundamental need of any community is an adequate supply of biologically and chemically safe, palatable water of good mineral quality. If the present rate of growth of population and industry continues, the quality of natural water will deteriorate and it will be difficult to guarantee the high quality of bulk water supply for domestic uses. With the development of new chemical compounds day by day for an ever-increasing demand of the consumer market, and with the increasing use of chemicals in agriculture and industry, new micro-pollutants are finding their way into natural water courses.

Although it is possible that by treatment the mineral quality and palatability of water can be improved, additional treatment cost to remove trace chemicals and high TDS will be high. It would be difficult and costly to produce very high quality bulk water for all domestic purposes from such sources.

It has been reported[1] that of the water used in households in England only about 3.2 percent is used for drinking and cooking and about 9.6 percent is used for dishwashing and cleaning. About 35 percent is used for personal hygiene; another 35 percent is used for toilet flushing, and 10 percent is used for laundering. The remainder is used for gardening and car washing. This analysis of various household uses indicates that about 87 percent of household water does not require water of very good quality with respect to TDS and trace chemical contaminants which would cause objection if ingested for a long time.

However, if it is assumed that only a small fraction (about 13 percent) of household water must be of the quality of drinking water, the volume of water to be treated by expensive sophisticated treatment processes would be small enough to allow economy in treatment. The remaining nonpotable portion of the domestic water would be biologically safe and supplied through a separate distribution system.

Haney and Hamann[2] made a rational comparative study of conventional and dual water systems. The objective of the present study is to develop a mathematical model to evaluate the technical and economical feasibility of dual supply systems for two hypothetical British towns using twelve alternative schemes of treatment and supply.

PROJECTED WATER DEMAND

In this study the planning period was taken as 1971 to 2001. The demands on public water supply for domestic and industrial uses are assessed separately. Instead of projecting the total demands of past years, in this study the contributing factors are separated into per capita domestic demand, per capita industrial demand, and population growth.

By regression analysis of past domestic water consumption data of nine British towns, the best-fit equation for the per capita domestic demand index percent is given by:

$$100\,ID_t = 67.24 + 1.23\,t^{1.0786} \tag{1}$$

in which $100\ ID_t$ = per capita domestic demand index (percent) in the year t; t = number of years after the year 1950. Similarly, the best-fit equation for the per capita industrial demand index (percent) has been developed as:

$$100\,IT_t = 63.85 + 1.314\,t^{1.0888} \tag{2}$$

in which $100\ IT_t$ = per capita industrial demand index percent in the year t after 1950.

Combining Equations (1) and (2) and giving proper weighting for domestic and industrial demand, per capita total demand index percent can be approximated as:

$$100\,I_t = 65.95 + 1.26\,t^{1.0826} \tag{3}$$

The value of I_t for the year 1971 is 1.00.

By regression analysis of past population data of various towns, the best-fit equation for population index percent is obtained as:

$$100\,IP_t = 82.65 + 0.826\,t \tag{4}$$

After assessing separately the growths of population and per capita water demand, the total water demand projection for a town can be obtained by combining per capita water demand with population:

$$Q_t = POP_{71}\,(187.10 + 3.57\,t^{1.083})\,(0.827 + 0.00827\,t)\,, \tag{5}$$

in which Q_t = total water demand in t-th year after 1950 in million liters; POP_{71} = population in the year 1971 in thousands.

COST FUNCTIONS

To develop mathematical models for conventional and corresponding dual supplies, the capital costs and O & M costs of various units of treatment and distribution as functions of flow are required. Cost data for various units of treatment and distribution which are valid for England have been taken from the literature[3,4] and updated and formulated in mathematical functions valid for 1971, the base year in this study. All the various components considered in this study are divided into two groups as treatment and distribution and are listed with useful life periods in Table 1.

Unit No.	Unit Component	Useful Life years
1	River Intakes	30
2	Impounding Reservoir	60
3	Conventional Treatment	30
4	Chlorination Equipment	15
5	Contact Tank	40
6	Wells	15
7	Activated Carbon	15
8	Electrodialysis	15
9	Pumping Mains	30
10	Pumping Stations	15
11	Service Reservoirs	40
12	Distribution Mains	30

Table 1. Useful Life Periods of Components.

Capital cost (y) and O & M cost (Y) functions of various treatment units valid for 1971 are given in Tables 2 and 3, respectively. Costs are expressed in British Pounds (£ 1 = \$2.07) and flows (Q) are expressed in million liters per day.

Unit No.	Treatment Unit	Capital Cost Functions for 1971*
1	River Intakes	$y_1 = 3{,}830\ Q^{0.931}$
2	Impounding Reservoir	$y_2 = 274{,}673\ Q^{0.516}$
3	Conventional Treatment	$y_3 = 41{,}120\ Q^{0.781}$
4	Chlorination Equipment	$y_4 = 257\ Q$
5	Contact Tanks	$y_5 = 1{,}167\ Q^{0.723}$
6	Wells	$y_6 = 3{,}910\ Q^{0.874}$
7	Activated Carbon	$y_7 = 65{,}000 + (3{,}500 + 42.5d)\ Q$, d = dosage (mg/L)
8	Electrodialysis	$y_8 = (7.78\ \mathrm{TDS} + 5{,}070)\ Q + 11{,}275$, TDS = TDS in raw water (mg/L)

*Costs are in pounds (£1 = \$2.07). Q = plant size in million liters/day capacity.

Table 2. Capital Cost Functions.

Unit No.	Treatment Unit	O & M Cost Functions for 1971*
1	River Intakes	$Y_1 = 651\ q$
2	Impounding Reservoir	$Y_2 = 27.5\ q^{1.35}$
3	Conventional Treatment	$Y_3 = 1{,}635\ q$
4	Chlorination Equipment	$Y_4 = 36.5\ q$
5	Contact Tank	$Y_5 = 0.42\ q$
6	Wells	$Y_6 = 930.75\ q + 173.9\ q^{1.431}$
7	Activated Carbon	$Y_7 = 1{,}785\ q/(q - 8.5)^{0.107}$
8	Electrodialysis	$Y_8 = 8{,}088\ q^{0.9}$

*Costs are in pounds/year (£ 1 = \$2.07). q = production per day in million liters.

Table 3. O & M Cost Functions of Treatment Units.

Distribution System

From available literature[4,5], the total installed capital cost of a pipeline can be expressed as a function of diameter:

$$C = KD^{m} \tag{6}$$

in which C = cost of pipeline per meter length and D = diameter of pipe in millimeters. For England (1971) in open areas the values of K = 0.0067 and m = 1.272; for built-up areas K = 0.0134 and m = 1.272. The O & M cost of water distribution mains of a town in England has been found to be £76 per kilometer per year.

Pumping station capital cost has been expressed in the literature[4,5] as a function of installed power:

$$y_{10} = k_{10}\,(\mathrm{kW})^{m_{10}} \tag{7}$$

in which y_{10} = capital cost of pumping station, kW = installed power in kilowatts, and k_{10} and m_{10} are parameters of the cost function. For England (1971) the value of k_{10} = 523.0 and of m_{10} = 0.785 when y_{10} is expressed in pounds.

Operating costs of a pumping station including the costs of labor, electricity and maintenance for England (1971) are a function of operating head as:

$$Y_{10} = (13.61\,H + 379.0)\,q \tag{8}$$

in which Y_{10} = pumping station O & M cost in £ /year; q = average daily pumping rate in million liters per day, H = operating head, in meters.

From a regression analysis of the cost data from England and considering a 24-hour storage in the service reservoir, the capital cost function for a service reservoir can be expressed in terms of design flow:

$$y_{11} = k_{11}\,Q^{m_{11}} \tag{9}$$

in which y_{11} = capital cost in pounds: Q = design flow in million liters/day; k_{11} = 19,169 and m_{11} = 0.723. Operating costs of the service reservoir in pounds can be expressed as a function of design flow in million liters/day as:

$$Y_{11} = 20\,Q\ . \tag{10}$$

DISTRIBUTION SYSTEM ANALYSIS

Considering the total cost of a pumping system consisting of capital costs of pumps and pipelines and their O & M costs, a mathematical model of a pumping system has been developed in order to optimize the total cost in seeking the least cost diameter for the pipeline[5]. The cost functions for pumps and water mains valid for England (Equations 6, 7, and 8) have been used to obtain the most economical diameter as a function of flow:

$$D_{opt} = k_9\,Q^{m_9} \tag{11}$$

where k_9 and m_9 are functions of cost function parameters, flow equation parameters and interest rate. For this study, it has been found that

$$D_{opt} \propto Q^{0.464} \tag{12}$$

combining with the cost function of capital cost of the pipeline (Equation 6):

$$\text{Capital Cost of Optimum Main, } y_c \propto Q^{0.59} \tag{13}$$

Pumping Mains

To compare the optimum capital costs of a conventional (single) system and a dual system of supplies, consider a total flow of Q, potable flow of rQ, and nonpotable flow of (1 - r) Q. For the same lengths of mains, the cost of mains in a single system Y_S is proportional to $Q^{0.59}$; in the dual system Y_D is proportional to $Q^{0.59}\,[r^{0.59} + (1-r)^{0.59}]$. The ratio of cost of mains in a dual system and a single system can be given as:

$$Y_D/Y_S = r^{0.59} + (1-r)^{0.59} \qquad (14)$$

Gravity Mains

The costs of single and dual mains under the same hydraulic gradient have been compared. Using the Hazen-Williams Equation for pipe flow and pipeline cost function (Equation 6), the cost of a gravity main with constant hydraulic gradient can be expressed as proportional to $Q^{0.483}$. The ratio of cost of gravity mains in a dual system and a single system can be expressed as:

$$Y_D/Y_S = r^{0.483} + (1-r)^{0.483} \qquad (15)$$

Distribution mains from the service reservoir to the consumers have been assumed to be under a constant hydraulic gradient.

MODEL FORMULATION

Mathematical models of dual and conventional water supplies considering 12 different treatment systems (Table 4) have been developed. Two typical hypothetical British towns with 1971 populations of 100,000 (Town A) and 500,000 (Town B) have been considered to develop treatment system and distribution system models of dual supply. Total treatment and distribution costs of conventional supply and of dual supply for all 12 treatment systems have been formulated, and the difference of treatment and distribution costs between single and dual supplies for all the 12 systems have been calculated. In formulating the mathematical models, the parameters such as potable-to-total-flow ratio, r; interest rate, i; annual capital cost increase rate, c_c; and annual O & M cost increase rate, c_o, are considered as variables.

System No.	Single Supply		Dual Supply			
			Potable		Nonpotable	
	Source	Treatment	Source	Treatment	Source	Treatment
TS1	Surface[1]	Storage + Conventional + Chlorination[3]	Surface	Storage + Conventional + Chlorination	Surface	Storage + Chlorination
TS2	Surface	Storage + Conventional + Carbon bed + Chlorination	Surface	Storage + Conventional + Carbon bed + Chlorination	Surface	Storage + Conventional + Chlorination
TS3	Surface	Storage + Conventional + Electrodialysis[4] + Chlorination	Surface	Storage + Conventional + Electrodialysis + Chlorination	Surface	Storage + Conventional + Chlorination
TS4	Ground[2]	Electrodialysis + Chlorination	Ground	Electrodialysis + Chlorination	Ground	Chlorination
TS5	Surface	Storage + Conventional + Carbon bed + Chlorination	Ground (limited)	Chlorination	Surface	Storage + Conventional + Chlorination
TS6	Surface	Storage + Conventional + Electrodialysis + Chlorination	Ground (limited)	Chlorination	Surface	Storage + Conventional + Chlorination
TS7	Surface	Storage + Conventional + Electrodialysis + Chlorination	Ground	Electrodialysis + Chlorination	Surface	Storage + Conventional + Chlorination
TS8	Surface	Storage + Conventional + Carbon bed + Chlorination	Ground	Electrodialysis + Chlorination	Surface	Storage + Conventional + Chlorination
TS9	Ground	Electrodialysis + Chlorination	Ground (Separate limited)	Chlorination	Ground	Chlorination
TS10	Surface	Storage + Conventional + Carbon bed + Electrodialysis + Chlorination	Surface	Storage + Conventional + Carbon bed + Electrodialysis + Chlorination	Surface	Storage + Conventional + Chlorination
TS11	Surface	Storage + Conventional + Electrodialysis + Chlorination	Ground	Electrodialysis + Chlorination	Ground	Chlorination
TS12	Surface	Storage + Conventional + Carbon bed + Chlorination	Ground	Electrodialysis + Chlorination	Ground	Chlorination

[1] All surface source systems would include river intakes and pumping.

[2] All ground source systems would include boreholes and pumping.

[3] Chlorination includes chlorination equipment and contact tank.

[4] For electrodialysis a reject ratio of 20 percent is assumed.

Table 4. Various Treatment Systems Considered for Dual Supply.

Basis of Formulation

The econo-mathematical models for all the systems have been developed on the following basis: 1) The models represent hypothetical new British towns and therefore are general theoretical models rather than specific ones. 2) Cost functions are derived from the literature and provide only approximate costs; they are indicative, not definitive. They are certainly not applicable, without adjustments, to specific cases. 3) The quality of water from the single-supply source is assumed to be the same as the potable supply in a dual-supply system. 4) Quantities of water required are obtained by projecting per-capita domestic and industrial demand; however, the rate of growth has been kept as a variable so that other rates of growth can also be incorporated in the model. 5) A leakage loss of 15 percent has been assumed. 6) Administrative costs have been included in all cost functions.

In comparing the costs of single supply and corresponding dual supply, all the costs incurred during the planning period (1971-2001) have been converted to the present value of the base year (1971). If some of the treatment or distribution units have residual design life remaining at the end of the planning period, the residual values of the units have also been considered as assets in the calculation of the system cost.

Treatment Systems

The present values of all capital and O & M costs incurred during the planning period of all treatment units have been calculated using corresponding cost functions for design flow, Q; potable flow rQ; and nonpotable flow (1-r)Q. As the design period for chlorination equipment, activated carbon treatment, electrodialysis and pumps has been assumed to be 15 years, the design flow for these units has been taken as the water demand in the year 15 years after installation. The design period for all other units has been assumed to be the same as that of the water demand at the end of the planning period.

The operational cost functions for various units have been related to the variable water demand, Q_t, during the planning period. The present value of the total operation cost of a unit throughout the planning period has been obtained by summation of the present values of all yearly operational costs, which may be expressed as

$$Y_{pv}(TN1)_{Q,t} = \sum_{t=1}^{30} Y_t(TN1)_{Q,t}\left(\frac{1+c_o}{1+i}\right)^t \qquad (16)$$

in which $Y_{pv}(TN1)_{Q,t}$ is the present value of the total O & M costs of treatment unit number 1 when the flow variable is Q_t; $Y(TN1)_{Q,t}$ is O & M cost in the t-th cost in 1971 figures; c_o is the rate of increase of O & M cost per year; and i is rate of interest per year. In the dual supply system, flows through the potable line would be rQ_t, and through the nonpotable line would be $(1-r)Q_t$. Equation 16 can be used to calculate the present value of O & M costs.

The calculation of present value of capital cost of a treatment unit which will be constructed 15 years from the beginning of the planning period can be expressed as

$$PVy_{15}(TN1)_{Q,30} = y_o(TN1)_{Q,30}\left(\frac{1+c_c}{1+i}\right)^{15} . \qquad (17)$$

in which $PVy_{15}(TN1)_{Q,30}$ = present value of the capital cost of treatment unit number 1, at a design flow at t = 30 years, which would be incurred 15 years from the base year; $y_o(TN1)_{Q,30}$ = the cost of the unit at base year price level; and c_c = rate of increase of

$$+ Y_t(TU13)_{(1-r)Q,t}) + \sum_{t=1}^{30} \left(\frac{1+c_o}{1+i}\right)^t [Y_t(TU12)_{rQ,t}$$

$$+ Y_t(TU12)_{(1-r)Q,t} + Y_t(TU10)_{rQ,t} + Y_t(TU10)_{(1-r)Q,t}$$

$$+ Y_t(TU11)_{rQ,30} + Y_t(TU11)_{(1-r)Q,30}] \quad . \qquad (21)$$

Equations 20 and 21 represent the total present value in pounds of all capital and operation costs of distribution systems during the planning period (1971-2001) in single supply and dual supply systems, respectively.

RESULTS AND DISCUSSION

The econo-mathematical models for single and dual supply for 12 treatment systems of total present costs of treatment and distribution of water were solved using a high-speed computer for various potable/total flow ratios (r values), interest rates (i values), capital cost increase rates (c_c values), operational cost increase rates (c_o values) for A-type (base population 100,000) and B-type (base population 500,000) towns. The computer output comprises total treatment costs, both capital costs and O & M costs, and total distribution costs for all the 12 systems. The cost advantage of dual supply over single supply, DEL, is expressed by the difference of total present value costs of single and dual systems in pounds sterling.

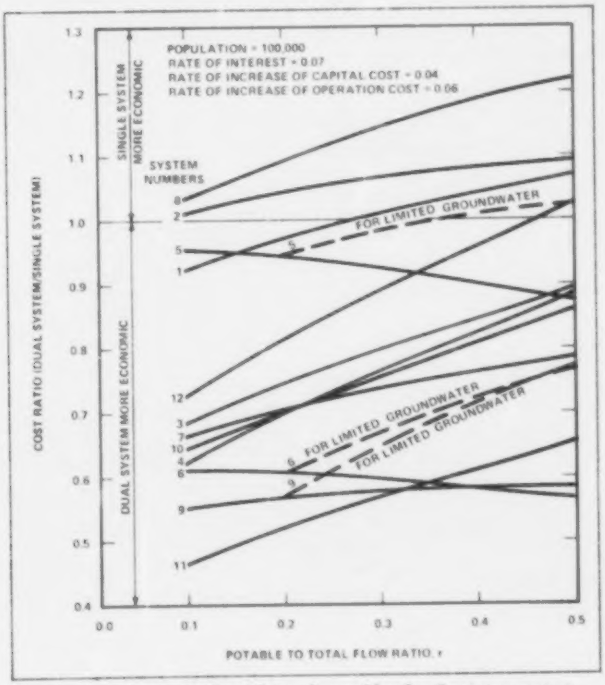

Figure 3. Cost Ratio of Dual to Single System versus Flow Ratio.

The cost ratio of a dual system to a single system has been plotted with potable to total flow ratio, r, for 12 treatment systems in Figure 3. The cost advantage of dual supply over single supply (DEL values) has also been plotted with interest rate, i, and operation cost increase rate, c_o, in Figures 4 and 5, to show the sensitivities of i and c_o to DEL values.

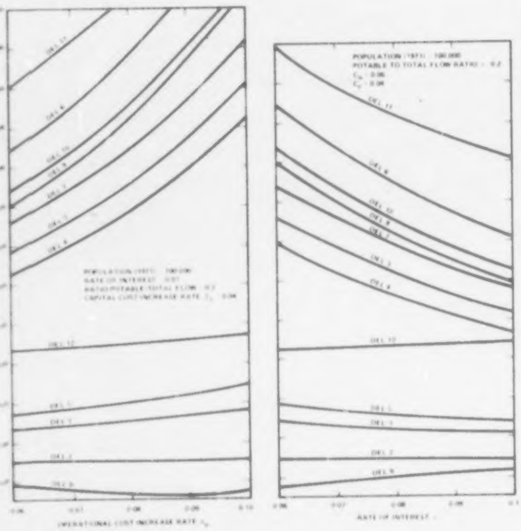

Figure 4. DEL versus i. Figure 5. DEL versus c_o.

For Treatment System No. 1, where the potable supply requires complete conventional treatment and the non-potable supply requires only chlorination, and dual system is found to be more economical than a conventional system if the potable requirement is less than 29 percent of the total.

Where the raw water source contains high TDS and demineralization is required (Treatment Systems 3, 4, 6, 7, 9, 10 and 11), a dual system is more economical than demineralization of the entire supply. Where a limited supply of high quality ground water is available, a dual system is more economical than a conventional system.

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capital cost per year. Equation 17 can be rewritten for potable and nonpotable flow in order to incorporate the cost of a dual supply system.

The present value formulations of capital and O & M costs of treatment of single and dual supply of 12 treatment systems of Table 4 have been made. A schematic diagram of Treatment System No. 1 is shown in Figure 1 and a corresponding investment diagram during the planning period is shown in Figure 2.

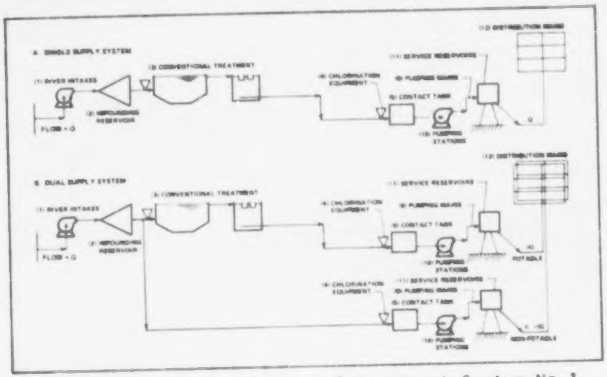
A. SINGLE SUPPLY SYSTEM
(1) RIVER INTAKES
(2) IMPOUNDING RESERVOIR
FLOW = Q
(3) CONVENTIONAL TREATMENT
(4) CHLORINATION EQUIPMENT
(5) CONTACT TANK
(9) PUMPING MAINS
(10) PUMPING STATIONS
(11) SERVICE RESERVOIRS
(12) DISTRIBUTION MAINS
Q
B. DUAL SUPPLY SYSTEM
POTABLE
NON-POTABLE

Figure 1. Schematic Diagram of Treatment System No.1.

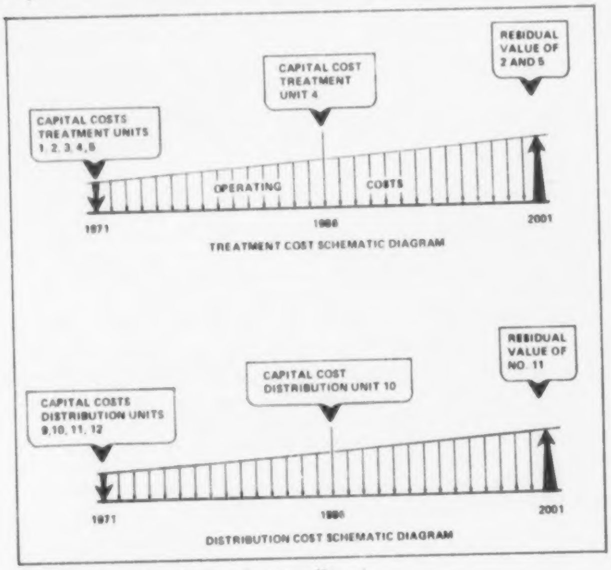
CAPITAL COSTS TREATMENT UNITS 1, 2, 3, 4, 5
CAPITAL COST TREATMENT UNIT 4
RESIDUAL VALUE OF 2 AND 5
OPERATING
COSTS
1971
1986
2001
TREATMENT COST SCHEMATIC DIAGRAM
CAPITAL COSTS DISTRIBUTION UNITS 9, 10, 11, 12
CAPITAL COST DISTRIBUTION UNIT 10
RESIDUAL VALUE OF NO. 11
1971
1986
2001
DISTRIBUTION COST SCHEMATIC DIAGRAM

Figure 2. Treatment System No. 1.

The total present value formulations of capital and O & M costs of Treatment System No. 1 for single and dual systems are given as follows:

(i) Single Supply

$$y_{pv}(S1S) = y_o(TN3)_{Q,30} + y_o(TN4)_{Q,15} + y_o(TN5)_{Q,30}$$

$$+ PVy_{15}(TN4)_{Q,30} + RVy_{30}(TN5)_{Q,30}$$

$$+ \sum_{t=1}^{30} \left(\frac{1+c_o}{1+i}\right)^t \left[Y_t(TN3)_{Q,t} + Y_t(TN4)_{Q,t}\right.$$

$$\left. + Y_t(TN5)_{Q,t}\right]. \qquad (18)$$

in which $y_{pv}(S1S)$ = present value of total treatment costs of System No. 1 in single supply.

(ii) Dual Supply

$$y_{pv}(S1D) = y_o(TN3)_{rQ,30} + y_o(TN4)_{rQ,15} + y_o(TN5)_{rQ,30}$$

$$+ y_o(TN4)_{(1-r)Q,15} + y_o(TN5)_{(1-r)Q,30}$$

$$+ PVy_{15}(TN4)_{rQ,30} + PVy_{15}(TN4)_{(1-r)Q,30}$$

$$- RVy_{30}(TN5)_{rQ,30} - RVy_{30}(TN5)_{(1-r)Q,30}$$

$$+ \sum_{t=1}^{30} \left(\frac{1+c_o}{1+i}\right)^t [Y_t(TN3)_{rQ,t} + Y_t(TN4)_{rQ,t}$$

$$+ Y_t(TN5)_{rQ,t} + Y_t(TN4)_{(1-r)Q,t} + Y_t(TN5)_{(1-r)Q,t}] \qquad (19)$$

In which $y_{pv}(S1D)$ = present value of total treatment costs of system No. 1 for dual supply.

In Equations 18 and 19 the treatment costs of treatment units 1 and 2 have not been included, since the costs of these units in both the systems are equal. In a similar way the treatment cost formulation of all the 12 treatment systems has been developed and incorporated in the model.

Distribution System Formulation

The distribution system formulation of all the 12 treatment systems will be the same. The total costs of a distribution system consist of capital costs and operation and maintenance costs of pumping mains, pumping stations, service reservoirs, gravity mains and yearly addition of gravity mains in the distribution system. All the costs involved during the planning period have been converted to present value and formulated as follows:

Single supply

$y_{pv}(DSS)$ = Present value (1971) of total distribution cost in a single supply system.

$$= y_o(TU9)_{Q_m,30} + y_o(TU10)_{Q_m,15} + PVy_{15}(TU10)_{Q_m,30}$$

$$+ y_o(TU11)_{Q,30} - RVy_{30}(TU11)_{Q,30} + y_o(TU12)_{Q,30}$$

$$+ \sum_{t=1}^{30} Y_t(TU13)_{Q,t} \left[\left(\frac{1+c_c}{1+i}\right)^t - \frac{t}{30}\left(\frac{1+c_c}{1+i}\right)^{30}\right]$$

$$+ \sum_{t=1}^{30} Y_t(TU10)_{Q,t} \left(\frac{1+c_o}{1+i}\right)^t$$

$$+ \sum_{t=1}^{30} Y_t(TU11)_{Q,30} \left(\frac{1+c_o}{1+i}\right)^t$$

$$+ \sum_{t=1}^{30} Y_t(TU12)_{Q,t} \left(\frac{1+c_o}{1+i}\right)^t \qquad (20)$$

Dual Supply

$y_{pv}(DSD)$ = Present value (1971) of total distribution cost in a dual supply system.

$$= y_o(TU9)_{rQ_m,30} + y_o(TU9)_{(1-r)Q_m,30}$$

$$+ y_o(TU10)_{rQ_m,15} + y_o(TU10)_{(1-r)Q_m,15}$$

$$+ PVy_{15}(TU10)_{rQ_m,30} + PVy_{15}(TU10)_{(1-r)Q_m,30}$$

$$+ y_o(TU11)_{rQ,30} + y_o(TU11)_{(1-r)Q,30}$$

$$- RVy_{30}(TU11)_{rQ,30} - RVy_{30}(TU11)_{(1-r)Q,30}$$

$$+ y_o(TU12)_{rQ,30} + y_o(TU12)_{(1-r)Q,30}$$

$$+ \sum_{t=1}^{30} \left[\left(\frac{1+c_c}{1+i}\right)^t - \frac{t}{30}\left(\frac{1+c_c}{1+i}\right)^{30}\right] (y_t(TU13)_{rQ,t}$$

DATA COLLECTION FOR WATER QUALITY MODELING IN THE OCCOQUAN WATERSHED OF VIRGINIA

T.J. Grizzard, C.W. Randall, and R.C. Hoehn
Department of Civil Engineering
Virginia Polytechnic Institute and State University
Blacksburg, Virginia

ABSTRACT

A large-scale water quality monitoring program has been instituted to provide runoff water quality data in sufficient detail to facilitate calibration of a predictive model using pollutant washoff theory. The sampling program involves the installation of automatic sampling stations, automated chemical analysis of collected samples, and use of the EPA STORET system as a data management tool.

BACKGROUND

The Occoquan Reservoir lies on the southern periphery of the Washington, D.C. Metropolitan area. The contributing drainage basin comprises portions of six political jurisdictions as shown in Figure 1. Impounded in 1957, the reservoir today provides a useful storage of 9.8×10^9 gallons (3.7×10^{10} liters), and serves as the raw water supply for an estimated 600,000 customers in suburban Virginia. In the late 1960's, rapid development began to occur immediately above the headwaters of the reservoir, creating the unusual situation of having an urbanizing area directly upstream of a water supply impoundment. Currently, eleven secondary waste treatment plants in the Manassas-Western Fairfax County area discharge about 8 MGD (3×10^7 LPD) of treated wastewater to the surface waters of the basin.

Observations of the reservoir in the period 1968-1970 showed advancing signs of cultural eutrophication, characterized by periodic blooms of nuisance algae and accompanying low raw water quality at the Fairfax County Water Authority Treatment Works (1). Unusual steps, including the application of massive quantities of copper sulfate to the reservoir body, hypolimnetic aeration of the intake area and the addition of activated carbon slurry to the treatment flow, have been taken to date to assure the continued use of the impoundment as a raw water supply.

In an effort to solve the above problem, the Virginia State Water Control Board, in July 1971, issued a "Policy for Waste Treatment and Water Quality Management in the Occoquan Watershed" (2). Two major articles of that document required that existing waste discharges be consolidated and treated by a "state-of-the-art" advanced wastewater treatment (AWT) plant in the Manassas area, and that a continuous, basin-wide water quality surveillance program be instituted to evaluate the effectiveness of the AWT processes in reducing pollution problems in the reservoir. As a corollary to this, it was necessary for the monitoring program to initiate efforts to quantify and project the sources of diffuse pollutant yields in the stormwater runoff from urban and agricultural lands in the basin.

POLLUTANT WASHOFF

At present, most stormwater quality models (3, 4, 5) assume first order kinetics in simulating the washoff of pollutants from the land surface during runoff events. That is to say, the amount of any pollutant removed from the ground surface during a given time interval is proportional to the quantity present at the beginning of the time interval, as in the following equation:

$$\frac{dx}{dt} = -kx \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; [1]$$

where,

x = Pollutant Load (mass)
t = Time
k = Decay Coefficient (time $^{-1}$)

This relationship has been used widely as a predictive tool in modeling the washoff of pollutants that accumulate on the land surface. It does not account for pollutant runoff yields associated with soil erosion and, therefore, has its best pure application in the simulation of washoff from urban (impervious) land uses. It has, however, been shown to be a reasonable tool to use in the simulation of applied materials washoff from agricultural lands (4, 5). The inclusion of such items as fertilizers, crop residues, and animal wastes in this category greatly enhances the suitability of the relationship for use in agricultural areas.

Upon integration and applying appropriate boundary conditions equation [1] becomes:

$$X_0 - X = X_0 \, (1 - e^{-kt}) \quad . \; . \; . \; . \; . \; . \; . \; [2]$$

where,

X_0 = Initial pollutant load on ground surface (mass)
X = Pollutant load remaining at time, t
$X - X_0$ = Pollutant load washed off at time, t

Empirical evaluation of the constant, k, is essential to the application of equation [2] to the simulation of pollutant runoff loads. One approach is to assume that k varies in direct proportion to the rate of stormwater runoff according to:

$$k = br \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; [3]$$

where,

r = runoff rate for watershed (depth/time)

In order to evaluate b, it is necessary to make an assumption about the quantity of pollutant removed from the ground surface by a given runoff event. One approach has been to assign a 90 percent removal to a uniform runoff of 0.5 inch/hour on an impervious surface and 50 percent on pervious surfaces (4). This results in the following relationships:

$$X_0 - X - X_0 \, (1 - e^{-4.6rt}) . \; . \; . \; . \; . \; . \; [4]$$

for impervious surfaces (4) and:

$$X_0 - X = X_0\ (1 - e^{-1.4rt}) \ldots\ldots [5]$$

for pervious surfaces (4).

The runoff rate, r, may be satisfactorily predicted using a number of hydrologic models currently available (6, 7).

MODEL CALIBRATION

The previous equations allow the investigator to compute the quantity of a given pollutant washed off the ground surface during a runoff event, and allow, therefore, the determination of runoff-borne pollutant loads and assessment of their impacts on receiving waters downstream.

Such a tool, however, can be only as good as its calibration from real-time observation of water quality data during runoff events. The key factor in the model is the successful estimation of X_0, the quantity of pollutant on the ground surface at the initiation of runoff. The determination of X_0 is based upon the assumption of a constant rate of accumulation of a given constituent on the ground surface during the dry days preceding a runoff event. Figure 2 is a dimensionless representation of the assumed relationship between storm runoff, pollutant loading, and pollutant-loading graph are approximately the same. This observation has been reported numerous times in the literature (8, 9, 10) and is descriptive of most types of surface runoff except where the so-called "first-flush" phenomenon is observed in heavily storm-sewered areas (9). The bottom portion of the figure is a representation of the washoff function described by equation [2] rearranged to read:

$$X = X_0 EXP(-kt) \ldots\ldots\ldots [6]$$

The discontinuities in the function occur at those times when runoff ends and begins anew, respectively. The linear portions between those times are representative of the assumed-to-be-constant "pollutant accumulation rate" used to arrive at X_0 for the next storm to occur. The length of the time axis between the beginning and end of an accumulation period is interpreted as the number of dry days between storms, as the length during decay periods is interpreted as the duration of a runoff event.

It may also be inferred from Figure 2 that:

$$X_{0i} = X_{t(i-1)} + \frac{\Delta x}{\Delta t}\,[t_i - t(i-1)] \ldots\ldots [7]$$

That is, that X_{0i} for any storm is determined by summing the quantity of pollutant remaining after the last storm and the product of the number of ensuing dry days and the accumulation rate, $\frac{\Delta X}{\Delta t}$.

The calibration procedure is as follows:

1. A data base consisting of pollutant loading graphs and hydrographs for a sequence of storm events in the watershed of interest is selected.

2. A pollutant loading curve for the initial storm event is plotted. X_0-X is taken to be the area lying under the curve. This value is substituted into the washoff equation [4] [5] along with observed values of "r" and "t" and a solution for X_0 is obtained.

3. A trial accumulation rate, $\frac{\Delta X}{\Delta t}$, is chosen.

4. The model is executed for a series of storms, the hydrologic and water quality data for which already exist. The simulated pollutant washoff loads are then compared to the observed loads.

5. Sequential adjustments are made in the assumed accumulation rate until the simulated runoff loads match the observed ones.

6. The above procedure is repeated for each constituent to be simulated.

SAMPLING METHODOLOGIES

Data to be used for runoff water quality model calibration must necessarily be more detailed than that generated for periodic ambient water quality assessments. It is necessary to have sufficient information to calculate a total pollutant load for each runoff event used in the calibration. Such information necessarily must consist of flow and concentration data of varying detail. A discussion of the methods of sampling commonly used and commentary on their suitability follows. The assumption is made that flow and concentration measurements are made at the same frequency.

Grab Sampling

Historically, most stream water quality surveys have been made using grab sampling. The unmodified procedure has little use in runoff model calibration, however, because it generates a pollutant load descriptive of only one instantaneous condition and takes no cognizance of the variation in load along the pollutant loading graph. A load calculated from the product of a single flow and concentration and extended to include the entire period of runoff could differ tremendously from the actual load (10).

Simple Composite Sampling

In this method, sample aliquots of equal volume are withdrawn at intervals during a runoff event and are composited into one volume for analysis. The flow used to estimate total load is the mean of the instantaneous flows at the times of sample collection. This method assigns equal weight to each aliquot of the composite; consequently, those portions taken during periods of relatively high flow affect the final concentration less than they should. Depending on the relationship between concentration and flow, the true load may be either over-estimated or under-estimated.

Flow-Weighted Composite Sampling

In this method, variable size aliquots of sample are composited, with the volume of each being directly proportional to the flow occuring at the time of sampling. The total load then is computed from the mean flow and the flow-weighted mean concentration of the composite sample. The technique gives an excellent estimate of Total Pollutant Load during a runoff event if sampling time intervals are small (3). Even so, the next method of sampling to be discussed offers a better means of characterizing pollutant variation in runoff.

Sequential Discrete Sampling

While this method is the most expensive option for sample collection, because it requires the most analytical work, it also provides the greatest flexibility for checking the calibration of the washoff equation [2]. In this method, discrete samples are withdrawn at numerous points on the storm hydrograph. The samples are separately analyzed and the results coupled with flow data taken at the time of collection in order to produce a number of instantaneous pollutant loads during the period of runoff. Plotting these loads on a time axis produces an approximation of the general pollutant loading graph illustrated in Figure 2. As the interval between samples decreases, the adherence to the actual loading curve increases (as do analytical costs). The quality of the total load estimate made by computing the area under the plotted pollutant loading curve is matched only by that from the flow weighted composite method. The latter, however, does not allow the investigator to determine the shape of the loading curve, and, therefore, prevents him from making any observations regarding the relationship between pollutant concentration and hydrograph shape. Additionally, knowledge of the pollutant loading curve makes it possible to consider making more refined estimates of the coefficient b in equation [3].

Table I shows a set of runoff data collected by the Occoquan Watershed Monitoring Laboratory (OWML) from a tributary to Bull Run near Manassas, Virginia. The summary loadings (a through e) contrast the total load estimates that would have been made on the set of data using each of the sampling methods discussed against the total load calculated by computing the area under a "smooth-curve" of pollutant load vs. time. As may be seen, the single grab sample method gives the worst estimate, errors ranging from -88 to +79 percent. The use of the simple composite method produced errors from -5 to +15 percent, depending upon the size of the composite. The flow weighted composite method produced an error of -7 percent using the smaller number of samples and an error of less than one percent using the full number of samples. The sequential discrete sampling method also produces the same total load estimate as the all sample flow weighted composite. As stated above, however, it also allows the investigator to determine the morphology of the loading curve.

FIELD APPLICATION OF SAMPLING PROCEDURES

OWML currently operates automatic sampling stations at seven locations in the Occoquan Watershed as shown on Figure 1. The drainage areas of the stations and the general land use types are given in Table II. All the streams on which sampling stations are located are perennial and, therefore, base loading measurements are necessary to enable the definition of runoff loads. Base loads are determined by sampling at all stations on a weekly basis during dry weather flow. Experience has shown that is not feasible to rely on individuals to occupy sampling sites during runoff events because such events are so unpredictable. During high intensity, short duration rainfall, runoff may commence immediately, and if sampling is not initiated concurrently, a significant portion of the pollutant load may be missed entirely. This happens in heavily sewered areas in particular, due to the liklihood of observing the so-called "first-flush" effect. It appears, then, that satisfactory sampling of runoff events necessitates the use of automatic equipment for sample collection, storage, and measurement of flow. Many automatic sampling devices are now available commercially, but most were initially developed for wastewater sampling; therefore, careful evaluation of proposed units should be made prior to purchase to assure that adequate performance may be expected in retrieving runoff samples. In particular, attention should be given to the recovery of suspended solids because of the propensity of stormwater runoff to carry some materials of higher specific gravity than those normally carried in wastewater discharges. Consideration should be given to heating the installation if normal operation during winter months is desired. Remote sampling equipment has decreased in size and increased in performance in recent years, and units are now available that may be easily carried by one person, and yet perform as well as the earlier, more bulky models. Recent studies (11, 12) have evaluated commercially available equipment and given guidelines for sampler selection. In general, an acceptable remote sampler will meet the following criteria:

1. Be weathertight and battery powered.
2. Be capable of collecting a minimum of 24 discrete samples of not less than 500 ml each and storing them in an insulated container.
3. Be capable of actuation from an external signal or from an internal clock at varying intervals.
4. Be capable of lifting a sample against a suction head of 10 feet at a minimum transport velocity of 3 feet per second (.91 m/s).
5. Have the capacity to distribute a single sample among several containers as it may be necessary to add differing preservatives for subsequent analytical work to be performed.
6. Be capable of conducting a pre- and post-sample purge of the intake hose to prevent clogging and cross-contamination of samples.
7. Have an intake that can be placed sufficiently high above the channel bottom to avoid sampling suspended bed load.

In performing runoff studies, equally important as obtaining representative samples is the measurement of flow, because no loading calculations may be made without reasonably accurate discharge measurements. In perennial streams with adequate natural control, flow measurements may be readily obtained by calculations involving velocity (obtained with a current meter) and cross-section measurements (13). In small watersheds that drain only during storm events, and lack an adequate natural constriction, the installation of some artificial control structure may be necessary. Several types of weirs and flumes have been used with success in studies of the hydrology of small watersheds (14). In urban storm sewer systems, the use of the Manning formula to compute flow as a function of stage provides the simplest method of obtaining flow data. However, selection of the value of the roughness coefficient, n, in all but the most recently installed conduits, poses a difficult problem. As the sewer ages, growths and other depositions cause changes in the surface roughness which can only be approximated when selecting a value for n. If the Manning formula is to be used with success, an indirect measurement of n for the reach of sewer in question should be made. "Calibration" of a sewer may be readily accomplished by using chemical gaging techniques to develop a reliable set of discharge-depth of flow relationships. The values of flow thus obtained may be used to compute a valid n for use in the Manning formula. Lithium chloride has recently been shown to be a satisfactory tracer for use in chemical gaging studies (16). In any case, adequate flow measurements are essential and obtaining them should be given high priority.

Figure 3 is a schematic of a permanent sampling installation operated by OWML. Flow measurements are obtained by making a continuous record of stream stage and comparing it against a stage-discharge curve prepared previously. The water-stage recorder wheel holds bar magnets spaced at 0.25 foot (.076M) intervals along its circumference. As the stream stage rises or falls, the magnets passing over a stationary reed switch provide a momentary contact closure that actuates the sampler in the adjacent building causing samples to be taken at known stage increments. Samples are stored in separate containers until retrieved and transported to the laboratory for analysis.

ANALYTICAL TECHNIQUES

As stated earlier, the sequential discrete sampling method is both the most reliable and the most expensive for generating accurate estimates of total load and loading rates. The greatly increased analytical workload is the major reason for higher costs. Because the number of samples to be analyzed may be an order of magnitude higher than that required in a program where samples are composited, consideration should be given to adopting automated analysis procedures where possible. Runoff samples from stations are retrieved as soon as possible following a storm. Table III shows the analytical schedule considered to be necessary to adequately describe the impact of nutrient and organic material runoff loads on receiving waters.

Nitrogen and Phosphorus

Nitrogen determinations are performed on both whole samples and aliquots filtered through 0.45 micron membrane filters (with the exception of nitrite and nitrate, because these forms are anionic and do not readily adsorb on suspended soil particles). For all other forms of nitrogen and phosphorus, the two types of analysis are necessary to determine the distribution between particulate and dissolved phases. This distribution is critical when considering the ultimate water quality impact of nutrient loadings.

Organic Matter

Two measures of organic loading are utilized: Biochemical Oxygen Demand (BOD) and Total Organic Carbon (TOC). The BOD determinations are made either in static bottles or with a manometric apparatus. TOC measurements are made in parallel with BOD analyses and correlations established with a view to using TOC as a "real-time" parameter for the measurement of organic matter.

Data Storage

All data are currently stored in the EPA STORET data management system. Data are reduced in the laboratory, coded, and stored on a biweekly basis. The system software greatly simplifies the computations required to develop pollutant loading information. By using the "MEAN" or "PLOT" routines (16), the investigator is able to obtain instantaneous load vs. time information in either tabular or graphical form. Upon integrating the loading curve by numerical or planimetric procedures, and using the proper scale conversions, it is possible to obtain the total storm load from the area lying beneath the curve.

SUMMARY

The Occoquan Watershed Monitoring Lab has established a network of automatic water samplers at locations on tributaries to the Occoquan Reservoir. Samplers are programmed to collect and store sequential discrete samples at increments of rising and falling stream stage during runoff. When combined with concurrent flow data, analysis of such samples allows the generation of pollutant loading graphs. Such loading data are invaluable in the precise calibration of most mathematical models used to simulate pollutant quantities in surface runoff. For calibration, the measured rates of constituent accumulation will be sequentially varied to achieve agreement in loadings between observed and simulated storms.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the contributions of the political jurisdictions participating in the Occoquan Watershed Monitoring Program. Additionally, the authors wish to acknowledge the tireless efforts of the OWML staff members without whom operation of the monitoring program would be impossible.

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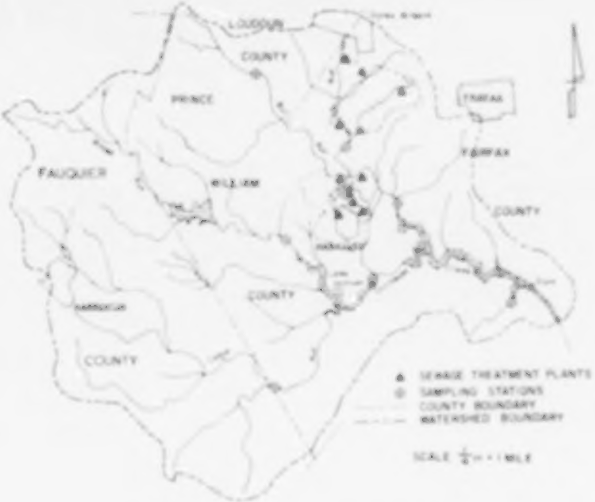
LOUDOUN
COUNTY
PRINCE
WILLIAM
FAUQUIER
COUNTY
FAIRFAX
FAIRFAX
COUNTY
MANASSAS
COUNTY
SEWAGE TREATMENT PLANTS
SAMPLING STATIONS
COUNTY BOUNDARY
WATERSHED BOUNDARY
SCALE ½" = 1 MILE

Figure 1. Occoquan Watershed

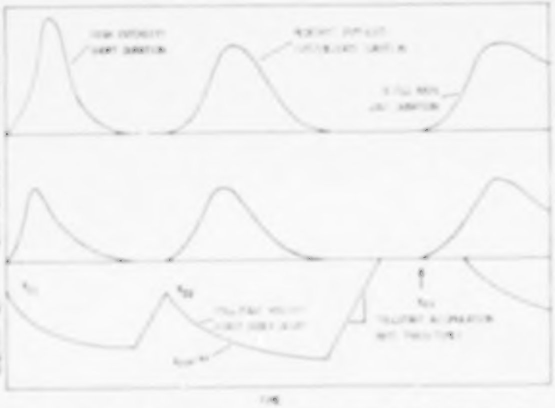

FIGURE 2. [illegible]

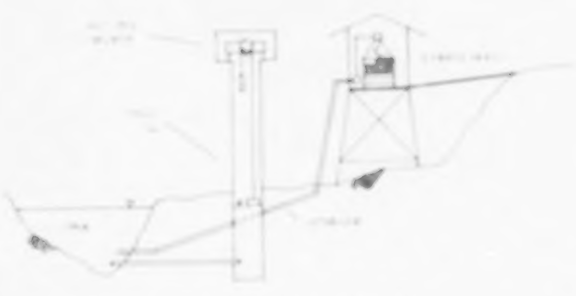

FIGURE 3. [illegible]

TABLE I

[illegible]

Sample No.	Date/Time	Flow (l/s)	Total P (mg/l)	Sample No.	Date/Time	Flow (l/s)	Total P (mg/l)
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]				

a. [illegible]
b. [illegible]
c. [illegible]
d. [illegible]

e. [illegible]
f. [illegible]
g. [illegible]

TABLE II

[illegible]

STATION	DRAINAGE AREA	MAJOR LAND USE
1. [illegible]	[illegible]	[illegible]
2. [illegible]	[illegible]	Mixed Urban
3. [illegible]	[illegible]	[illegible]
4. [illegible]	[illegible]	[illegible]
5. [illegible]	[illegible]	[illegible]
6. [illegible]	[illegible]	Mixed Urban
7. [illegible]	[illegible]	[illegible]

TABLE III

Analytical Schedule For
Non-Point Studies

PLANT NUTRIENTS	ORGANICS
Total Phosphorus	BOD
Ortho Phosphorus	TOC
Total Soluble Phosphorus	
	SOLIDS
Total Kjeldahl Nitrogen	
Soluble Kjeldahl Nitrogen	Total Suspended
Total Organic Nitrogen	
Soluble Organic Nitrogen	
Nitrite + Nitrate	

WATER SUPPLY SYSTEMS PLANNING, MANAGEMENT AND COMMUNICATION THROUGH AN INTERACTIVE RIVER BASIN SIMULATION MODEL

Robert A. Hahn
Civil Engineer, Systems Analyst

U.S. Army Corps of Engineers, Ohio River Division
Cincinnati, Ohio

Summary

The Washington Metropolitan Area Water Supply Study initiated the development of a unique river basin simulation model designed to be incorporated into an open planning process. The model is a flexible, user oriented tool suitable for a number of different purposes. It has been used to educate Corps personnel in the intricacies of the Washington Area water supply system and to evaluate a number of water supply device alternatives. Potential uses include public demonstration of the complexity of the existing water supply system, evaluation of social, economic, or environmental impacts of water supply alternatives, the modeling of operational rules and as a "real-time" decision tool to show the effects of operational management decisions on all parts of the system.

Introduction

The water supply simulation model described in this paper was developed as part of the Northeastern United States Water Supply (NEWS) Study.[1] This study was authorized by Congress[2] in response to the mid-60's drought throughout most of the Northeastern United States, for the purpose of preparing plans to meet long-range water supply needs of that area. The Washington, D.C. Metropolitan Area (WMA) was identified as one of several critical areas of the northeast urgently requiring additional water supply capacity. Detailed planning began in the WMA in the fall of 1972 with an extensive "open planning program" designed to find out as much as possible about the alternative water supply solutions available and the preferences of the local public and private agencies and individuals.

It became obvious by the spring of 1973 that the problem was too complex for hand analysis of the various planning alternatives. Meta Systems Inc.[3] was asked to develop a tool which would allow the study team to examine a large range of alternative solutions without the time-consuming and error-prone drudgery of analyzing each variation by hand. Many aspects of the study could not be modeled, but those amenable to an analytic approach and within the limits of modeling technology were included. This paper will limit itself to those aspects of the study incorporated in the model. The complexity of the problem is due to the combined effect of three separate factors: the unusually complicated nature of the existing water supply system; the social, economic, and environmental issues discovered during the open planning process which broadened the way in which the problem must be solved; and the range of alternative engineering solutions proposed.

Existing Water Supply System

The study area was defined as the portion of Maryland, Virginia, and Washington, D.C. within the Washington Area SMSA which includes seven counties, several incorporated cities, 3,000 square miles, 2.9 million people using 390 million gallons of water per day, and the nation's capital. The area's water is supplied by two river basins, the Patuxent, which is small (930 square miles), well regulated, and located entirely in Maryland, and the Potomac, which is large (14,700 square miles), unregulated, and located in four states and the District of Columbia. The major supply source is the Potomac River, which has large seasonal variations, highly random daily variations, and drought stages of less than six percent of the average. Since maximum daily withdrawals have already exceeded minimum flow in the Potomac, and since most, if not all, future source development will be in this basin, supply analysis becomes a problem in time and frequency. The question asked is not only how large are the deficits, but also how long, how often, and at what probability.

Two of the three major water suppliers in the study area presently use this source to supply 65 percent of the region's needs, and the third expects to use the river in the immediate future. Two other sources, reservoirs on the Patuxent and Occoquan Rivers, are also used to provide portions of the region's needs. These independent sources are only minimally interconnected, which raises the question of deficit locations. These questions, deficit location, probability, frequency, and magnitude are very important to the analysis of the existing system and evaluating the proposed improvements. They are also very difficult to answer as they require statistical processing of a large amount of data.

Social, Economic, and Environmental Issues

During the early "open planning" stage of the study, several issues were developed which had to be considered in any water supply solution. Many of these issues, though relatively complex socially, politically, and institutionally, were simple from an analytic point of view. An example is the interrelation of water and wastewater management. Other issues, such as the environmental impact of reservoirs, are also complex analytically and can only be analyzed quantitatively to the extent that functions can be derived which relate environmental parameters to water quantity. Finally, a large group of questions pertaining to overdesign and efficient resource use condense quantitatively to questions of planning not for the worst conceivable drought but for some lesser drought defined in terms of magnitude, duration, location, and frequency of shortage. Not only had this question never been seriously considered by water planners before, but existing literature and analytic techniques are not capable of answering the question to everyone's satisfaction.

Range of Alternative Solutions

The broad range of water supply technologies being considered in the study added further analytical complications. These included a range of water conservation measures, interbasin transfers, the use of treated estuary and wastewater, groundwater, and local and remote reservoirs.

Model Conception and Design

The concept of the model was simple—answer as many of the above questions as possible. Furthermore, answer the questions in a manner that is believable, with a model that can be operated by any technically competent person; that has flexible input, operation, and output; and that can be operated in an open planning session involving the public, other agencies, or the study team. The difficulty in structuring, coding, calibrating, and finally documenting such a model should be obvious to any experienced model builders, but at the time of its proposal, no lesser model would satisfy the needs of the study team. The model design can be examined in six main categories: model structure, interactive features, nodal definition, hydrologic simulation, model output, and social, economic, and environmental parameters.

Model Structure

The model is structured around a collection of 200 different nodes representing one of eighteen (18) node types at which water can be added, subtracted, or stored and a number of statistics can be collected. Figure 1 is a schematic illustrating the nodal chain and node types used. If, for example, the node were defined as a reservoir, (node type 1) natural and/or pumped inflow and outflow can occur, which will vary the storage within the reservoir accordingly. Statistics can be maintained of these variables, inflow, storage, etc., which are then outputs of the model. These nodes are strung together in a network which represents the region's water supply system. The model begins at the first node at time t = 0 and adds or subtracts waters from that node according to instructions coded for that node type and the values of user-supplied parameters such as reservoir capacity. The transaction is recorded, statistical counters are updated, and the model proceeds to the next node to be considered. This process is repeated until all 200 nodes have been processed at which time the model's clock is incremented by one and the program starts over again. The clock increments are either monthly or daily depending on the output desired. Decision switches automatically compare the flow or storage at a particular node with user-supplied maximum or minimum values, and adjusts the process sequence. For example, if the flow in the Potomac is less than a given minimum, and interbasin transfers are being modeled, the model will route through the Patuxent nodes before the Potomac nodes. At each node and time increment, the program will print out any parameter values desired for the nodes chosen. Finally at the end of the session, the user can choose to see statistics on any node and parameter of interest. A wide

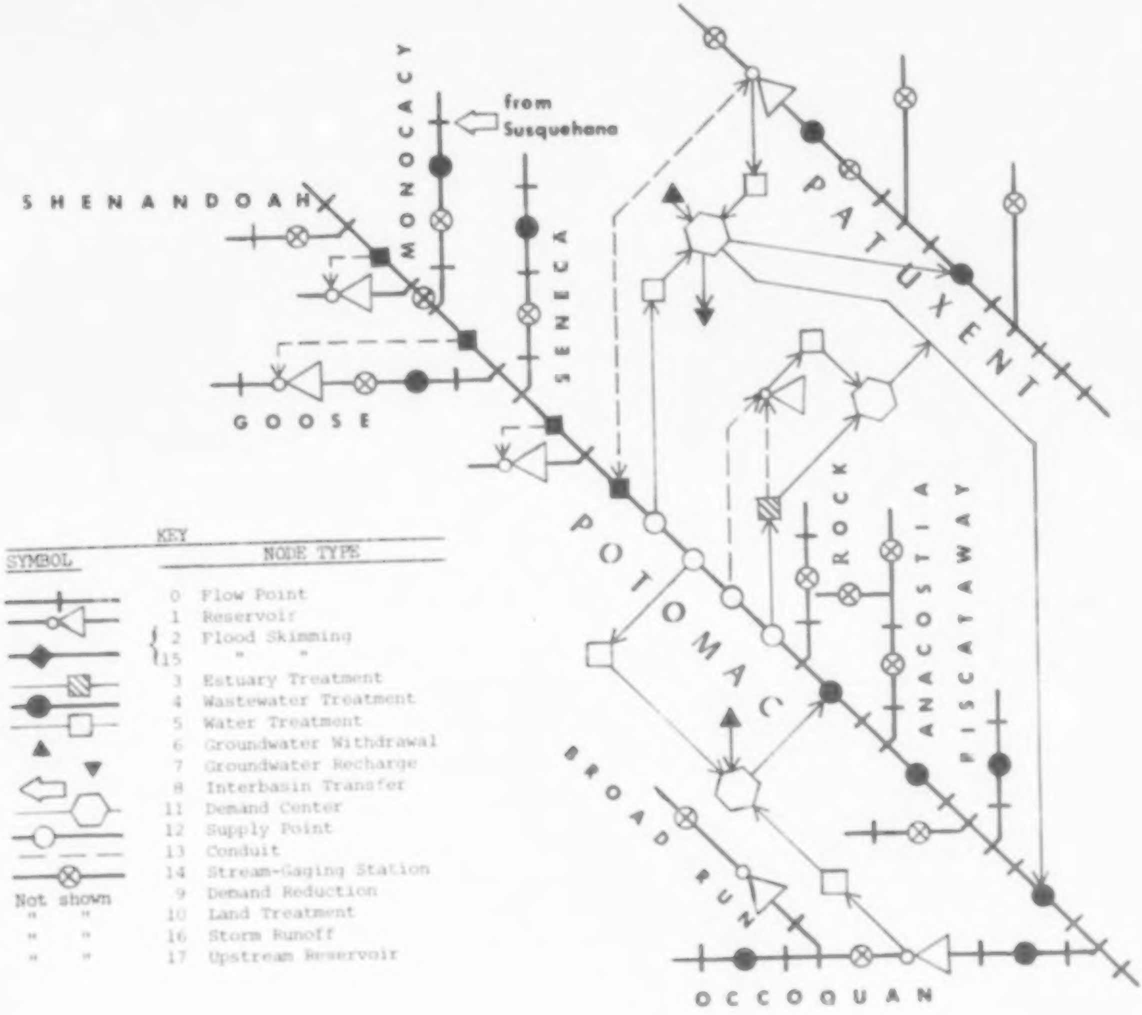
from
Susquehana
MONOCACY
SHENANDOAH
SENECA
PATUXENT
GOOSE
POTOMAC
ROCK
ANACOSTIA
PISCATAWAY
BROAD RUN
OCCOQUAN
KEY
SYMBOL
NODE TYPE
0 Flow Point
1 Reservoir
2 Flood Skimming
15 " "
3 Estuary Treatment
4 Wastewater Treatment
5 Water Treatment
6 Groundwater Withdrawal
7 Groundwater Recharge
8 Interbasin Transfer
11 Demand Center
12 Supply Point
13 Conduit
14 Stream-Gaging Station
Not shown
9 Demand Reduction
" "
10 Land Treatment
" "
16 Storm Runoff
" "
17 Upstream Reservoir

FIGURE 1. Schematic Illustrating Nodal Chain

variety of alternative events can be simulated by varying the nodal chain, the values of nodal parameters, and the switches used. This movement from node to node is controlled by the main program which calls subprograms to do the nodal transactions, to remember the transaction, to accumulate transaction statistics, and to control communication with the operator.

Interactive Features

A unique feature of the model is the way in which it communicates with the operator. This feature allows a technically trained person with some understanding of the system being modeled to learn to use the model in several hours. It also gives interested non-technical observers confidence that no trick is being performed and that they can interpret the results. It was incorporated into the model for the express purpose of planning in real time so that questions or alternative suggestions could be answered, or sets of results obtained, without time-consuming delays and difficult data manipulation problems associated with batch process programs. This feature required well over half of the coding (which consists of more than 3,000 Fortran lines) to be devoted to the interactive aspects of the program. It also consumes a large amount of computer resources during model operation, but its contribution in ease and flexibility of operation and in data handling and believability of results does add significantly to the value of the model as a planning tool.

Nodal Definition

Each of the eighteen node types shown in Figure 1 serve to represent a different type of water accounting. Many of the nodal types do not simulate the indicated function but merely act as a source or sink for water supply. The model does not simulate groundwater movements, for example, but merely supplies water on demand to a demand center up to a specified rate. Simulating the groundwater movement itself would have been difficult, impossible to calibrate, and unnecessary. Eliminating it greatly simplified the model without causing significant planning inaccuracies. The model is equipped with a data base called "BASE" which includes values for all the parameters necessary to simulate the existing situation. At the beginning of each session, the user has the opportunity to change the values of the parameters at the nodes to simulate the construction of a project. Impoundment A, for instance, does not presently exist and is represented in the data base as a reservoir with zero storage and pumping capacities. These capacities can be changed at the beginning of the run should the user wish to implement that reservoir and if the results are satisfactory, the revised data base can be saved for later use.

Hydrologic Simulation

Most of the model consists merely of accounting routines to subtract water from one node location, add it to another, and record the transaction. The one major exception, the driving force of the model, is the simulation of hydrologic events. Each of the rivers and tributaries modeled consist of a number of "dummy" and "routing" reaches connecting the river nodes together. Most of the reaches are "dummy" reaches, in which no routing or storage occurs and outflow of the upstream node becomes inflow to the node below it. The hydrology of the basin is simulated within the "routing" reaches. The flows recorded at eighteen U.S. stream-gaging stations are used to load the model with one of two historical water years (1930 or 1966) which were serious drought periods. Each of the "routing" reaches is related to one of the stream-gaging stations through drainage ratios, and the net water inflow in the region is allocated to the routing reaches as stream runoff or as stream inflow. Rivers act as natural reservoirs, with varying storage capacity which is also simulated in the routing reaches using Muskingum routing coefficients. The routing reach number, location, and routing coefficients were adjusted during calibration to accurately capture the response of the prototype.

Model Output

One of the major advantages of the model is the flexibility of output. At the beginning of each run the user can chose to observe the dynamic change in one or more parameters at one or more of the nodes, and these values will be printed at the terminal for each time period in the simulation. The feature is useful for observing changes in parameter values as they occur, and the relationship between values at a given time increment. This enables decisions on improvements for the next run and choices as to the final statistics desired. At the end of each run, a programmer can choose to see the statistics of any parameter, for any node. The statistics available are mean and standard deviation, a histogram of all events, and a trace of the events as they occur. The user may choose to see the output at the terminal or on a high-speed line printer. Normally, the user would choose to see a small portion of the output at the terminal, certain key parameters, for instance, and if the run were successful, he would ask to see all statistics printed on the high-speed printer for a permanent record and for later detailed study. The user may also write a message at the beginning of the printed output such as the date of the run, the users name, solutions used, and preliminary interpretation so that the output can be more readily used at a later date.

Social, Economic, and Environmental Parameters

The incorporation of social, economic, and environmental parameters is a feature built into the model that has not yet been used. At the present time, all output is limited to water quantity values measured as a rate (mgd) or a volume (bg). Many social, economic, and environmental factors related to water supply solutions can be described as functions of water quantities. For example, the region's economic growth is in part related to deficit probabilities, the cost of pumping water is directly related to the volume pumped, and certain environmental parameters in the estuary can be described in terms of the volume of fresh water flowing into the estuary. The model is designed to incorporate relationships such as these and is capable of generating these values and related statistics so that social, environmental, and economic impacts of any water supply decision can be at least partially simulated. To utilize this capability, the appropriate functions relating these impacts to water quantity must be provided.

Model Calibration

The value of any model depends on the confidence one has in the accuracy of its output, which can only be obtained by calibrating the model relative to the prototype for a range of conditions. Establishing the model's performance is particularly important when new modeling concepts are being used. It is seldom convenient to calibrate an entire model satisfactorily and in our case it was impossible because no complete, consistent system-wide data base exists. It is unlikely that such a set will ever be collected because the model imitates extreme events (droughts) for which one must wait on nature for the appropriate sampling conditions and because it predicts water supply system failures, which presumably will never be allowed to happen. It was, however, possible to calibrate four critical areas of the model independently to obtain an estimate of the accuracy of the entire model. These are streamflow routing, generation of streamflow gage records, generation of daily demand records, and the accounting procedure which moves water from one part of the system to the other. In each of these areas, excellent results were obtained giving an overall estimate of model accuracy at better than 90 percent, which far exceeds the requirements for a region-wide water planning model.

Streamflow Routing

Accurate imitation of drought conditions in a free-flowing stream requires an adequate procedure for computing instream storage with respect to time. The Muskingum three-coefficient equation

$$O_i = C_0 I_i + C_1 I_{i-1} + C_2 O_{i-1} \qquad (1)$$

was used to perform the routing where C_0, C_1, and C_2 are routing coefficients and are a function of travel time, routing period, and inflow-outflow weighting factors. These coefficients are difficult to obtain, particularly for drought conditons, since they are sensitive to stream bank conditions and river stage. Obtaining these coefficients (and in the process, calibrating this part of the model) could only be done by comparing computer-generated and observed streamflow during low flow conditions. The stream gage records and water production records of the water supply utilities were obtained for October 1970. The consultant then varied the number of river reaches and the storage coefficients to optimize the reproduction of the observed record by the generated record. The resultant streamflow simulation satisfactorily imitates the prototype with the critical flow parameters, low flow, mean flow, and temporal response within 10 percent, 4 percent, and 7 percent respectively, of the observed values.

Streamflow Generation

The primary input parameter of the model is stream gage records from eighteen locations in the region. The flow in each river reach is a function of inflow and outflow (change of storage) and runoff which are natural occurrences, and withdrawals and discharges which are manmade. The natural occurrences are determined through drainage area relationships from the stream-gaging records. Most of the gaging stations did not have records for the 1930 drought period, though fortunately the most significant gages did, and all records had one or more data gaps. Because the model simulated daily events, it was necessary to have a complete daily record for each gage for any historical or synthetic drought year modeled. Several established generating techniques were tried to complete incomplete records and for synthetic generation. These were found unacceptable because they could not adequately describe daily phenomena (which is highly skewed) or else they could not capture drought statistics satisfactorily. A procedure was found using the log normal distribution with skew unspecified for filling gaps in the record. The algorithm for filling the gaps used serial correlation for the longer records and cross-correlation for the shorter records based upon correlation coefficients for the portions of the records which overlap. This procedure was considered adequate to complete the records, but was not considered appropriate for use in a stochastic generator as it tended to distort serial correlation. Confidence in the completed historical records was gained in the process of completing the records.

Synthetic Demand Generation

The purpose of all planning simulation models is to predict the future behavior of existing or proposed systems. In this case the future is represented by the projected annual water demands, which must be supplied to the model. In order to use these demands in a daily flow model, it is necessary to modify the demands to reflect cyclic seasonal and random daily phenomena before they can be used to generate meaningful daily storage statistics. This requires a demand generator that takes annual demand for nineteen demand nodes and develops daily values for those nodes without distorting any of the meaningful demand statistics. Conceptually, this is a much simpler task than streamflow generation, as significant historical demand records are maintained at all the water supply utilities and satisfactory results were obtained relatively quickly using well established analytic techniques. However, few of the records were readily available and none in machine-readable form, which greatly increased the labor required to perform the task. We are confident that the demand generator will accurately generate daily demands in the model because of the accuracy with which it can duplicate historical demand patterns.

Accounting Procedure

Calibrating the accounting procedure which moves water from one part of the system to another is simple though time consuming and consists merely of evaluating the printed output of all parameters at all nodes for each time period under a number of given situations. The model was found to faithfully account for water movement about the system, neither losing or creating water, and moving it from location to location in the amount and the time expected. A fundamental constraint to the model was that its clock increment was daily which required that all water transfers be in multiple units of days. The time of travel (pumping distances) of pressurized water supply mains are small, significantly less than one day, so it was assumed that water transfer could occur from one part of the system to another instantaneously. Wastewater flows, however, which travel by gravity over greater distances, have varying travel times from location to location within the system. This was simulated by delaying wastewater return to the system by one day. Neither of the assumptions, that pressurized flow takes zero days to travel and that unpressurized flow takes one day, should cause significant errors.

Model Use

The purpose for which a model is developed and the way in which it is used when finished do not always correspond. This model has not yet been used in an "open planning" session to illustrate the intricacies of the water supply system or to experiment with alternative solutions. Nor has it been used to develop statistics about the location, duration, magnitude, frequency, and probability of deficients. It has also not been used to evaluate the proposed final alternative solutions. Time and money constraints, information delays, changing roles and approach of the team towards the study, and other unforeseen and uncontrolled events led to the completion of the model just shortly before the completion of the study. The credibility of both the model and the water supply study would have been enhanced had there been more time available.

Actual Model Use

The model was, however, extremely useful to the study, for in the process of developing the model much was learned about the proposed solutions, and the region itself, which would not have been learned otherwise. This is primarily because the model was not developed in one stage but was changed during the study as more was learned about the prototype, the model, and the solutions to be analyzed. At each stage of development, the model was operated for a range of system variations in order to learn as much as possible about the prototype, the model, and the solutions. Also, the difficulties encountered and overcome while obtaining a consistent correlated model required thorough analysis of data which revealed much about the system's hydrologic and demand patterns. For example, information gathered in the process of demand generation revealed that an analytic approach to system shortages is not possible with present mathematical techniques so that the location, magnitude, frequency, duration, and probability of the shortages must be obtained using sampling technique. This would consist of running the model hundreds of times with the same configuration to obtain statistical representation of the computed shortages. Resources did not permit this type of analysis but evaluation of the data revealed that some simplifying approaches would be appropriate. Another suprising result of the data analysis was that the demand patterns were highly predictable; indicating the possibility that conservation techniques may be more reliable than otherwise thought.

At each stage of the model, experiments were run to analyze the proposed solutions to determine their potential value and, if possible, obtain some parameter values that appeared promising. This analysis was done on a device-independent basis which does not indicate the interactions between devices in a system. This is not a concern with the final set of alternative solutions, however, since they would be implemented and operated with minimal device interaction. One of the preliminary experiments was to vary the regulation roles of the existing and proposed reservoirs. This led to the conclusion that these reservoirs could be used more efficiently, from a water supply standpoint than indicated by previous analysis.

Although this model was not used directly in plan formulation, information learned about the system and the alternative solutions led to the development of a simpler and more efficient, but also more limited, model which was used in plan formulation. Among other things, the simpler model considered the demand supply network in two nodes, Pototmac supply and demand and non-Potomac supply and demand. It was found in the early experiments on the water simulation model that satisfying these two demand supply nodes would be a satisfactory simplification of the prototype for the level of detail documented in the study report.

Potential Model Use

There are several potential uses for this model which have not been attempted and had not been considered when the model was developed. These became apparent as the alternative water supply solutions were formulated and as experience with the model was obtained. The model will be extremely useful as a public communications vehicle to educate the public on the existing water supply system and on the potentials for water supply development. Its use should decrease the problems of complicated and massive data bases necessary to document proposed projects and should increase the confidence that the public has in water supply plans. It can also be used by planning agencies as it was intended, as a planning tool to compare alternatives and determine the most appropriate solution to the water supply problem. Once the environmental, economical, and social parameter functions are included in the model, it will be valuable in determining the impacts of water supply solutions and can be used to keep the decision makers aware of the impacts of their decisions. It will assist in economic and environmental impact assessments, and could be used in cost-sharing and in the billing of utilities for the cost of regional water supply development and operation. Before the region can decide whether or not it will accept shortages, it must have a thorough understanding of the deficits that will occur. The model can be used to obtain these statistics. In its present form it would be extremely inefficient for this task but it can be converted into a batch process model relatively quickly and cheaply. Finally, many of the proposed solutions would be dynamically operated and the model could be used to establish the most efficient operating policies. Alternatively, it could be used to make operational decisions in "real time" predicting the consequences of any operational decision before that decision is made, greatly increasing the efficiency and decreasing the risk of operating those solutions.

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3. Consultant:
Meta Systems Inc., Cambridge, Mass.
Principal Investigator—Russell deLucia,
Model Coding—Lewis Koppel, Hydrologic
Simulation—Gerald Tierney, Water Demand
Analysis—Myron Fiering.

FUTURE DIRECTIONS IN URBAN WATER MODELING

Michael B. Sonnen, Prin. Engr.
Larry A. Roesner, Prin. Engr.
Water Resources Engineers, Inc.
Walnut Creek, California

Robert P. Shubinski, Vice Pres.
Water Resources Engineers, Inc.
Springfield, Virginia

Summary

A review was made for the Storm and Combined Sewer Section of the U.S. Environmental Protection Agency (EPA) concerning existing urban water mathematical modeling capability. From this review, gaps in needed modeling technology were identified, and a philosophical approach to filling those gaps was developed. Finally, a phased implementation program for developing the needed models was suggested.

Introduction

In 1974-75, a review was performed by Water Resources Engineers (WRE) for EPA's Storm and Combined Sewer Section concerning the state-of-the-art of urban water modeling. Moreover, WRE was then to recommend what model development work could be undertaken most feasibly in the next five years. The scope of the review was to include all the urban water subsystems, such as watersheds, water supplies, treatment, or water use, but the emphasis for obvious reasons was placed on storm and combined sewer problems and their modeling.

In this paper we outline our findings with respect to most of the urban water subsystems reviewed and suggest that inadequacies that continue to exist in problem-solving capability are more philosophical and scientific than numerical.

Subsystem Modeling Needs

Urban Watershed Hydrology

Urban hydrology received considerable attention from modelers as soon as computers became routinely available to them. This resulted in part because urban flooding and drainage problems were acute; damages were high and frequent. Moreover, analysts knew intuitively that the rational method for designing runoff facilities was theoretically weak and yet tedious in complex applications. So hydrographs, unit hydrographs, instantaneous unit hydrographs, systems of linear reservoirs, infiltration equations, Markov chains, and numerous other pieces of these and other puzzles were fed into the computer. Urban watershed models of quantity and quality have been the latest result. The recent attention to "nonpoint" sources of pollution has raised the importance of the urban runoff problem, while the ability to model the phenomena occurring, particularly the quality phenomena, has culminated for the moment with "dirt and dust" linkages that are theoretically weak, if empirically capable of calibration.

Water Distribution Systems

Water distribution systems have been analyzed with computer methods for years. Numerous utilities and private consultants have more than adequate versions of programs that balance heads and flows in these closed systems. Some, if not most, of the programs deal with numerically complicating system paraphernalia such as pressure reducing valves, variable speed pumps, and the like. The quality of water in these systems has not been included, however, and recent discussions of lead poisoning and carcinogenic substances in water supplies may draw more analysis attention to this important piece of the urban water system. Computerized, automatic operation is on the drawing boards as well, awaiting realization.

Water Use

To the writers' knowledge, the urban water use subsystem has never been rigorously simulated, in a cause-and-effect sense. The most elaborate model constructed appears to be MAIN-II, developed by Hittman Associates.[1] This model either accepts projections or makes its own for "independent" variables such as population density, values of dwelling units, and numbers of dwelling units in each value range. Among residential, commercial-institutional, industrial, and public-unaccounted sectors of the community, 150 separate water use categories can be projected. Other models include those of Schaake and Major,[2] and the "Data Management Systems" of WRE[3] and Montgomery-WRE.[4] All of these approaches to water use projection, however, depend on prior projections of independent variables, for example, population, per capita income, or water pricing policy. As such, they are all computerizations of effects and their trends, rather than models of water demand causes that simulate resultant effects.

Tihansky[5] and Sonnen[6] have each developed some quality-use-consumer-cost programs that calculate the added costs to homeowners or industries of excessive hardness or TDS in their supplies, but these accept demands as given and do not account for any diminution in projected unit demands if quality deteriorates or increases in use if quality is improved. In short, much more work could be done in simulation and economic modeling analysis of urban water use.

The water use subsystem is the most critical of all because it sets the quantity and quality demands for all upstream subsystems, plus it is the source of the quantity and quality loads imposed on all subsystems downstream.

Sewer Systems

Sewer design problems have been approached with models that adopt the steady-state "design flow" concept which obviously makes them more applicable to sanitary sewers than to storm sewers. Mathematical programming techniques have been used to discover optimal sizes, slopes, and—in rare cases—configurations of drainage networks. Fisher, et al.,[7] presented an integer programming formulation for the diameter-slope problem. In spite of finding a 10 percent cost savings over a traditional design method, the authors concluded that uncertainties in excavation costs, the dynamic nature of actual flows, and the arbitrary nature of velocity constraints detract considerably from the significance of the indicated saving. Argaman, et al.[8] have also considered optimal network configuration as well as pipe sizes and slopes. They found their dynamic programming approach to require amounts of computer time that severely limit the size of the sewer network that can be considered. The development of programming techniques for sewer design is relatively recent, and their application to real problems has not been documented.

Analysis models describe the performance of a given collection and conveyance system under given inflow conditions. Model output is usually in terms of flow rates, and possibly in terms of impurity concentrations over time at various points including at the system outfall. Brandstetter[9] has conducted a comprehensive review of the more sophisticated of these models. The initially developed hydraulic transport routine for EPA's SWMM model[10] is typical. Depending on the level of resolution needed to represent temporal variables and the pipe network, relatively coarse to highly sophisticated analytical models are available. SWMM is one of the more sophisticated (and expensive) of these models.

Water Resources Engineers has developed[11] and the Corps of Engineers has documented[12] a planning level model (STORM) in which continuous computer simulation (at hourly intervals) with historical rainfall records is used to predict the effects of various treatment and storage capacities on overflow quantities and quality. No consideration is given to the collection and conveyance system, however, and no cost relationships or optimizing algorithms have been included. A significant outcome of using this model, however, has been the emergence of the concept of the "design event" including a dry period for accumulation of pollutants on the watershed, as opposed to the purely hydrologic concept of a "design storm."

Waste Treatment

This subsystem received a flurry of modeling attention from early systems analysts. Most of this work was directed at optimizing the amount of waste treatment at various points along a stream, given a dissolved oxygen standard and the Streeter-Phelps equation. A later tack was taken to simulate waste treatment processes themselves. The majority of this work to date has been an exercise in programming the rules of thumb of sanitary engineering design, but some elucidation of process variables has resulted. A recent article by Christensen and McCarty[13] gives a hopeful signal that causes can be modeled fundamentally to predict effects rather than having to "predict" the answer from statistical analyses of the measured answers at 20 other plants.

Receiving Waters

Many, many programs to solve the Streeter-Phelps equation along streams were developed in the early 1960's. Link-node models for estuaries with dynamic hydraulic solutions were developed by 1965 for the Delaware estuary and for San Francisco Bay. Lake and reservoir temperature models and groundwater models followed by 1967-1969. In 1969-1971 the receiving water model called RECEIV was incorporated in the EPA SWMM model. During this period, the feasibility of modeling several aquatic trophic levels and their interrelated responses to ambient water quality was shown. This philosophy was eventually demonstrated for San Francisco Bay and Lake Washington. Since then many stream, estuary, and lake models have been developed and updated to include the "ecologic model" interrelationships.

Throughout the roughly 15-year history of modeling of receiving waters, the capabilities of the developed models have lagged behind the scope of the problems being faced by urban water management decision makers. Current problems specified for attention by the Water Pollution Control Act Amendments of 1972 include derivation of "wasteload allocations" for waters designated as "water quality class segments." Current ecologic models applied to this problem have proved helpful but less than completely satisfactory. The Safe Drinking Water Act of 1974 implies a need for a model to treat as many as 150 substances and their interactions.

Recommended Future Water Models

From its review of the state-of-the-art and its view of what is 1) most likely of early success, 2) most required in terms of pressing needs, and 3) most feasible in terms of EPA's research posture and wherewithal, WRE recommended[14] the following models receive development attention in the next 5 years:

Planning Models

1. A new and better watershed quality model.

2. A transport simulation capability in a planning model for storage/treatment/overflow evaluations (STORM-II).

3. Capability to simulate quality control or treatment processes in STORM-II.

4. A long-term (10-30 year) receiving water ecologic model.

5. An economics model for assessing users' water supply benefits and costs.

6. An economics model for assessing receiving water users' benefits and costs.

Design/Analysis Models

1. A solids deposition and scour capability in a hydraulically sound sewer transport model.

2. Dry-weather waste treatment simulation capability in a SWMM-type model.

3. Reclamation or reuse routing capability in a transport/treatment model.

4. Nonstructural runoff control simulation capability in a SWMM-type runoff module.

Operation/Control Models

1. Real-time control software for sewer systems.

2. Real-time spatially varied runoff prediction capability.

Modeling Philosophy

There are two points about modeling that our project has suggested may be more important to getting problems solved than the mere statement of a subsystem's set of unresolved technical circumstances. These are: 1) What are the consequences of poor communication between the developer of a model and its subsequent user? 2) What are the consequences of claiming to model a process when in reality we are managing somehow to reproduce the expected value of its output?

These problems are related to one another, and they may each be restatements of a more general riddle which could be stated, Why are we building all these models anyway? The quick, obvious answer is, We need them, just to perform all the computations for us, just to do the arithmetic involved in analyzing a basin-wide pollution problem over a 30-year period. Fine, that's answer enough. But such an answer implies 1) that the model developer and the user of the model's output each understand perfectly what arithmetic needs to be done, 2) that they are each confident that the computer is being told to do the correct arithmetic via the program, and, of course, 3) that the machine will do correctly what it is told to do. It seems to us that the last of these three assumptions is the only one worth betting on.

We conducted an informal survey of ten people, roughly half of which were model developers, academicians, researchers; the other half were model users, front-line water and waste managers, city officials, Federal data collectors, utility managers. With few exceptions we heard that communication between the developer of a model (computer program, really) and the subsequent user has been garbled at best. Invariably, a delivered program contains bugs, solves a slightly different and usually much simpler problem than the one(s) advertised, or simply will not function or execute with a different set of data.

There are many variations of the same communications problem. Often the delivered card deck and documentation reports do not clearly annotate the options available or assumptions implicit in the programs. Sometimes the mathematical statement of the general problem is far more precise than the data used to "verify" the model, and hence the program takes inordinate amounts of time and money to generate its highly approximated and questionable results. Saddest of all are the cases where the model developer and the ultimate user of the model's results, often the fellow who paid for the development, never communicated from the start; and the model developed addresses a problem the user never had, while his real problem is still unsolved.

Every developer of a model who has given his program to someone to use has heard these complaints. Ironically, he knew he would, and he let the program out of his hands anyway. Usually, he lets it go because the user bought it from him. But he knows, and the user cannot believe, that there will be problems with the very next application. Sometimes there is no excuse for this phenomenon, just as there is no excuse for somebody else's meatloaf not tasting like your mom's. They just are not the same; they were made differently even though they were called the same thing. Another reason it occurs is because the modeler knows from the start that he is setting out to approximate a solution to a theoretical problem with both an approximation of the theory and an approximation to the prototype water body. The model user or the user of the model's results views his problem, and the theoretical statement, as precise and infinitesimal. Almost invariably, the first application of a handed-over program is made to a problem that either 1) lies outside the range of applicability of the equations simplified in the program, or 2) requires a time step shorter than the model or its "theory" can accept. Highly qualified and experienced programmers make these mistakes just as neophytes do. The nondeveloper-user almost always expects a new program to be both more exact and more flexible than it is or was ever intended to be. Lastly, it occurs because modelers make mistakes.

Without question, improvements in model documentation and preparation of user's manuals can be made. The communications problems between modelers and subsequent users of their products are too numerous and well documented for simple sloppiness of explanation to continue. Responsibilities lie with both parties, however, and the tedious method of constant re-explanation between the developer and the subsequent user is the only failsafe procedure. A nondeveloper-user who picks up a program deck cold certainly is going to have problems with it, period.

So much for crossed wires and simple not hearing what the other fellow said. The more insidious problem is the "model" that both the parties accept but that is not a model at all. One of the respondents to our survey said, "... analysis of the results of the model run are the real key to application of any model." Right on. It is worth amplifying that computer printouts rarely if ever contain a singular answer to a real problem. The significant analysis leading to solution of a real problem starts when a successful run or set of runs ends. A model user has to be a qualified results analyst, or he is not a user at all. Getting a program to execute with data given in the format described in a user's manual is one problem, but interpreting the results is quite another and more important problem. To interpret the results correctly, of course, means that the user can correctly interpret the model's inputs and its general workings as well; and perhaps most importantly he must know and understand the particular water body, land surface, or treatment process being modeled. In other words, there is an onus on the user of the model or of its results to sort through the mass of modeled evidence to satisfy himself that either the model or the data are not quite correct or that the prototype could indeed behave in such a strange or unexpected way. If the results are just what he would have expected, he must still be able to determine whether the model and he were both right or he must be willing to accept the consequences.

For example, a computer program that predicts the suspended solids concentration in the effluent of a primary clarifier, from a relationship between overflow rate and the removal efficiency measured at 60 existing plants, is not a model of the behavior of a primary sedimentation tank. In a given situation, such a program may be adequate. It may even prove to have been right, once the 61st, "modeled" tank has been built. But the program was never written to simulate what would happen in the 61st tank, and the model developer could hardly be blamed if the 61st tank and its contents behaved quite differently. Unless, of course, he had claimed that he had modeled the sedimentation process, which he clearly had not. We might add, since currently there are so many people clamoring to use runoff quality models that exist today, that many of them have been built to "predict" qualities not on the basis of what happens on a watershed surface but on the basis of what has been measured to have resulted in the waters that ran off many other surfaces. There may be a big difference, and while some modelers may not even be aware that they're doing that, a user of the model must know it. In other words, many simulation models around today are designed to predict effects based on measured effects elsewhere; they are not designed to simulate causes which operate on input data to produce expectable effects. Future urban water models should be, but they are not now so designed because so much is still unknown about causative factors.

Future users, remember that despite the best intentions or dreams of the developer, a model is always imperfect. What you cannot forget is that a less than perfect representation of prototype systems is the goal of the process from the beginning.

Developers, remember that while adding more and more padding to a mannekin might make a better and better approximation of Requel Welch, it would be a delusion to expect Raquel to finally appear in the flesh. Both of you remember, it is fallacious to believe that an extra large bikini is a model of Raquel merely because, for at least part of the prototype, "it seems to fit."

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TRANSPORT MODELING IN THE ENVIRONMENT
USING THE DISCRETE-PARCEL-RANDOM-WALK APPROACH

S. W. Ahlstrom
Water and Land Resources Department
Battelle Pacific Northwest Laboratories
Richland, Washington

H. P. Foote
Water and Land Resources Department
Battelle Pacific Northwest Laboratories
Richland, Washington

Abstract

When formulating a mathematical model for simulating transport processes in the environment, the system of interest can be viewed as a continuum of matter and energy or as a large set of small discrete parcels of mass and energy. The latter approach is used in the formulation of the Discrete-Parcel-Random-Walk (DPRW) Transport Model. Each parcel has associated with it a set of spatial coordinates as well as a set of discrete quantities of mass and energy. A parcel's movement is assumed to be independent of any other parcel in the system. A Lagrangian scheme is used for computing the parcel advection and a Markov random walk concept is used for simulating the parcel diffusion and dispersion. The DPRW technique is not subject to numerical dispersion and it can be applied to three-dimensional cases with only a linear increase in computation time. A wide variety of complex source/sink terms can be included in the model with relative ease. Examples of the model's application in the areas of oil spill drift forecasting, coastal power plant effluent analysis, and solute transport in groundwater systems are presented.

Introduction

The fundamental principle upon which the Battelle Generalized Transport Model and all other mass transport models are based is the law of conservation of mass. This law can be expressed as:

The rate of change of mass concentration of chemical species k within a given control volume
= the net advective flux of the species k into the control volume
+ the net diffusive flux of species k into the control volume
+ the net rate of production of species k within the control volume (1)

A mathematical statement of Equation 1 is usually referred to as an equation of continuity. A general form of the continuity equation for a non-isothermal multicomponent fluid consisting of K chemical species can be written as[1]:

$$\frac{\partial \Gamma^k}{\partial t} = - (\nabla \cdot \Gamma^k \overline{v}) - (\nabla \cdot \overline{j}^k) + \phi^k, \qquad (2)$$

where:

$k = 1,2,3...K$

Γ^k = the mass concentration of species k

$\overline{v}$ = the mass average velocity of the fluid

$\overline{j}^k$ = the mass flux of k relative to $\overline{v}$ (diffusive flux)

ϕ^k = the net rate of production of species k within the control volume.

The addition of K equations of this kind gives the equation of continuity for a mixture. Each term of Equation 2 corresponds directly with the terms of Equation 1.

The term on the left-hand side of Equation 2 is referred to as the transient term. It may be interpreted as the total rate of change of mass concentration of species k at a point in space at a given instant in time. The mass concentration of any species is in general assumed to be a function of temperature, of time, and of spatial coordinates, as well as the concentration of all the other species present. The primary function of a transport model is to predict and quantify these changes in concentration as a function of time and location.

The first term on the right-hand side of Equation 2 is referred to as the advective term. This term represents a change in concentration of the system resulting from the gross movement of fluid in which species k is transported. The mass average velocity vector of the fluid mixture, $\overline{V}$, is a function of time, space, temperature, and the chemical composition of the mixture. If $\overline{v}$ is constant with respect to time, the flow field is said to be steady. For most applications to large scale environmental systems the assumption of a steady flow field is usually adequate only for short-term simulations. For most long-term simulations, the velocity field cannot reasonably be assumed to be constant.

The second term on the right-hand side of the equation of continuity is called the diffusive term. This term represents the change in concentration of the system resulting from the random molecular motion of each species in the mixture. The driving force of the relative mass flux, $\overline{j}^k$, can be concentration, pressure, temperature or other gradients. In many large scale environmental transport analyses the contribution of molecular diffusion is often very minor, but when eddy diffusion is coupled with molecular diffusion, this term may become much more significant. The rationale for the inclusion of eddy diffusion in this term is discussed below.

The last term in Equation 2 represents all internal mechanisms that tend to change the net amount of species k present in a control volume. The reactivity of a chemical system may be a function of temperature and any or all of the k mass concentrations in the mixture. Ideally this term should consist of a series of rate expressions which represent all known mechanisms by which species k can react with its immediate environment. Species for which ϕ^k is zero are referred to as conservative substances because they are neither created nor destroyed within a control volume.

Equation 2, as written, is a very general expression. It applies to both liquid and gaseous mixtures containing an arbitrary number of components in any ratio, reacting over a wide range of temperatures and pressures. Workable models are, by necessity, much more limited.

Simplifying Assumptions

Equation 2 serves as the starting point for the explanation of the assumptions that are present in the existing DPRW code. Simplifying assumptions were made for one or more of the following reasons:

1. A portion of the general equation, based on an analysis of the best available information, appeared to be relatively insignificant for the anticipated applications of the model.
2. The quality of existing data or additional data that can be reasonably obtained does not justify considering anything above a certain level of complexity.
3. To allow a numerical solution within reasonable economical constraints.

Each simplifying assumption will be denoted by sequential numbers enclosed in square brackets preceding the assumption as it appears in the text; i.e., the fifth assumption will be preceded by [5].

When advective fields are calculated or measured it is not practical to resolve the micro-advection patterns that are known to exist in nearly all large scale environmental flow systems. These turbulent flow patterns, often the primary mixing mechanism, achieve essentially the same result as diffusive processes only much more rapidly. In some respects, micro-advection phenomena, commonly called eddy or turbulent diffusion can be thought of as a random process, occurring on a larger scale, but having many characteristics in common with molecular scale diffusion. Because of these similarities, it has been the practice historically to [1] approximate this phenomena by including it with the molecular diffusion in the relative mass flux term, $\bar{J}$.

If it is assumed that [2] the relative mass flux can be adequately described by expressions having the form of Fick's First Law, then $\bar{J}$ can be expressed as:

$$\bar{J}^k = -\Gamma \bar{\bar{D}}_m^k \nabla w^k - \Gamma \bar{\bar{D}}_e \nabla w^k \tag{3}$$

where:

Γ = total mass density of the solution

$\bar{\bar{D}}_m^k$ = molecular diffusivity tensor

$\bar{\bar{D}}_e$ = eddy or turbulent diffusivity tensor

w^k = the mass fraction of species k (Γ^k/Γ)

The diffusivity tensors are in general functions of both space and time. If the molecular diffusivity is assumed [3] to be negligible with respect to the turbulent diffusivity and if [4] only the longitudinal components of the tensor are considered to be significant then Equation 3 can be reduced to:

$$\bar{J}^k = -\Gamma D \nabla w^k \tag{4}$$

where

D = longitudinal components of the eddy diffusivity tensor

The velocity distributions required for a transport simulation can be derived from a hydrodynamic numerical or physical model study, and/or a field measurement program conducted prior to running the simulation. The assumption inherent in this practice is that [5] the advection patterns are not dependent on the chemical composition or temperature of the solution, or in other words, the momentum, mass and energy transport processes are decoupled. This assumption is valid for systems that are not highly non-isothermal and which contain relatively low concentrations of contaminants.

Another assumption [6] considers the transporting medium (water) to be incompressible. This assumption is considered valid for most water mixtures that are not near the boiling point. The restriction to incompressible fluids causes the convenction term of Equation 2 to be simplified as follows:

$$\nabla \cdot \Gamma^k \bar{v} = \Gamma^k \overset{= 0 \text{ for incompressible fluids}}{\cancel{(\nabla \cdot \bar{v})}} + (\bar{v} \cdot \nabla \Gamma^k) = \bar{v} \cdot \nabla \Gamma^k \tag{5}$$

If all of the above assumptions are incorporated into Equation 2, and also assuming that [7] the total mass density, Γ, of the mixture remains relatively constant. The result is:

$$\frac{\partial \Gamma^k}{\partial t} = -(v \cdot \nabla \Gamma^k) + (\nabla \cdot D \nabla \Gamma^k) + \phi^k \tag{6}$$

Although this equation was developed from a mass balance point of view, it can also describe the transport of heat under appropriate circumstances. Starting with the law of conservation of energy, and making assumptions identical or analogous to those made above, one can derive an energy balance with the same functional form as Equation 6. Consequently, the transport of mass or heat can be calculated by the same numerical computation code.

Boundary Conditions

Boundary conditions for transport analyses can be specified quite simply. Four boundary types are defined:

1. Free Flow Boundary - any matter or energy transported across this type of boundary is assumed to have exited from the system.
2. Reflecting or No Flow Boundary - any component encountering this type of boundary is reflected back into the system.
3. Unconditional Sticking Boundary - any substance that comes in contact with this type of boundary will adhere to it.
4. Conditional Sticking Boundary - when matter comes in contact with this type of boundary it may adhere to the boundary or be reflected from it. The percentage of the coincident

matter that is allowed to stick is calculated from a predefined probability distribution function.

The Numerical Solution Algorithm

A system of matter can be viewed from two alternative frames of reference. The classical approach is to view the advection-diffusion processes from an Eulerian point of view, establishing the transport equation from a consideration of concentrations and flux of a continuum at fixed points in space. A quantity of matter can also be thought of as being comprised of a large number of discrete particles. Keeping this in mind, it is also possible to approach the transport problem from a Lagrangian viewpoint, focusing on the history of particle motions. To arrive at useful results, statistical properties of the motions have to be considered, so that this second approach may be labeled as "statistical", in contrast to the "phenomenological" method mentioned above.

Both of these approaches, if pursued, will yield Equation 2.[2] However, the viewpoint that is chosen to derive the transport equation has some very definite implications relating to possible numerical solution techniques. The phenomenological approach which views matter as a continuum suggests the application of finite difference or finite element numerical techniques. The statistical viewpoint suggests a different type of approach using a discrete particle, Lagrangian algorithm. This type of numerical scheme is used in the most recent version of Battelle Generalized Transport Model and is referred to as the Discrete-Parcel-Random-Walk method.

The basic device or tool employed by this technique is a hypothetical entity called the computational parcel. A quantity of matter or energy is represented as consisting of a finite ensemble of these parcels. Each parcel has associated with it a set of Cartesian spatial coordinates (x_p^n, y_p^n, z_p^n) and a set of discrete quantities of matter or heat $\xi_p^{k,n}$, where:

p = the parcel index (p = 1,2,3...P) where P is the total number of parcels used to represent a given quantity of matter.

k = the transported species index (k = 1,2,3...K) where K is the total number of constituents present in the system.

n = the time level index (n = 1,2,3...N) where N is the number of time increments to be computed.

For example, the location of parcel 3 after 5 time steps is (x_3^5, y_3^5, z_3^5). If the problem is concerned with 5 distinct constituents, this parcel would have associated with it 5 separate heat or mass quantities $\xi_3^{1,5}$, $\xi_3^{2,5}$, $\xi_3^{3,5}$, $\xi_3^{4,5}$, and $\xi_3^{5,5}$.

The DPRW transport code requires a velocity matrix describing the flow patterns of the transporting media as input data. The flow field is allowed to be a function of both time and space. The two spacial velocity components at the location of parcel "p", (u_p^n, v_p^n, w_p^n), can be interpolated from the surrounding matrix of values. The advective transport component is then computed by:

$$x_p^* = x_p^n + \Delta t^n u_p^n \qquad (7a)$$

$$y_p^* = y_p^n + \Delta t^n v_p^n \qquad (7b)$$

$$z_p^* = z_p^n + \Delta t^n w^n \qquad (7c)$$

where Δt is the time increment, and * denotes an intermediate or temporary value.

If a smooth continuous solution is desired the maximum value of Δt should be limited by the requirement that the maximum distance any parcel is transported must be less than or equal to the distance between data points in the velocity matrix.

The dispersive component for each parcel is then calculated by assuming that the parcels are subject to Brownian-like random motion resulting from turbulence present in the transporting medium. From statistical considerations it can then be shown that the root-mean-squared (rms) distance moved by a given parcel during the time, Δt, in three-dimensional isotropic space is

$$r_{rms} = \sqrt{6D\Delta t} \qquad (8)$$

where D is the eddy diffusivity which is proportional to the square of the "typical" eddy size.

The dispersive step size for an individual parcel is generated by:

$$r_d = [R]_0^z \qquad (9)$$

$[R]_0^z$ represents a random number in the range 0 - z where z must be chosen so that the rms value of all of the r_d generated is equal to the value specified by Equation 8. The random number generators available on most computer systems will return values in the range 0.0 - 1.0. The rms value of the set of all numbers output by a number generator of this type is given by Equation 10 if, in fact, the generator is truly random.

$$\left(\int_0^1 r^2 dr\right)^{1/2} = \left(\frac{r^3}{3}\Bigg|_0^1\right)^{1/2} = \frac{1}{\sqrt{3}} \qquad (10)$$

Assuming that an adequate random number generator of this type is available, dispersive step lengths with the appropriate rms distance can be generated by

$$r_d = \sqrt{3}\,[R]_0^1\,\sqrt{6D\Delta t} = [R]_0^1\,\sqrt{18D\Delta t} \qquad (11)$$

The new Cartesian coordinates of each parcel are then calculated by

$$x_p^{n+1} = x_p^* + r_d \cos(\theta)\sin(\phi) \qquad (12a)$$

$$y_p^{n+1} = y_p^* + r_d \sin(\theta)\sin(\phi) \qquad (12b)$$

$$z_p^{n+1} = z_p^* + r_d \cos(\phi) \qquad (12c)$$

where θ is a random angle from 0 - 2π and ϕ is a random angle from 0 - π.

Parcel "p" has thereby been transported by advection and diffusion mechanisms from (x_p^n, y_p^n, z_p^n) to (x_p^{n+1}, y_p^{n+1}, z_p^{n+1}) during time step "n". The trace of a parcel during this time step is illustrated in Figure 1.

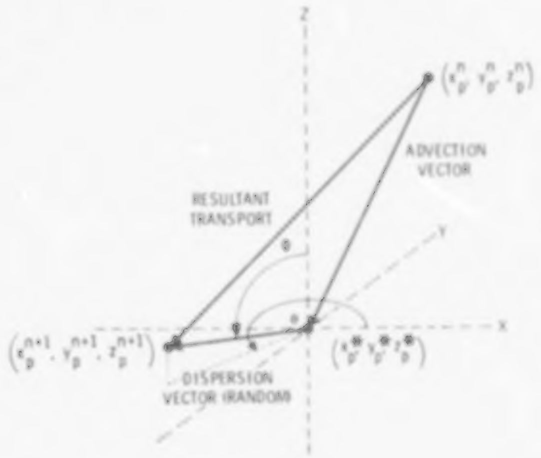

Figure 1. Vector Diagram of Transport Components

When this computation has been completed for every parcel in the system, a grid network can be superimposed upon the spatially distributed ensemble of parcels. The nodal points of the grid are labeled with i,j,ℓ indices where:

$i = 1,2,3....$ I = number of nodal points in x-direction

$j = 1,2,3....$ J = number of nodal points in y-direction

$\ell = 1,2,3....$ L = number of nodal points in z-direction.

The nodal points form the vertices for $(I-1) \times (J-1) \times (L-1)$ rectangular solids which are referred to as cells. Parcel "p" is said to lie within cell (i,j,ℓ) if

$$x_i \leq x_p^{n+1} < x_{i+1} \tag{13a}$$

$$y_j \leq y_p^{n+1} < y_{j+1} \tag{13b}$$

$$z_\ell \leq z_p^{n+1} < z_{\ell+1} \tag{13c}$$

The total amount of matter or energy within cell (i, j,ℓ) is computed by summing the $\zeta_p^{k,n}$ values for all parcels that lie within the cell for each species:

$$\zeta_{ij\ell}^{k*} = \sum_{\pi=1}^{\eta_{ij\ell}} \left(\zeta_p^{k,n}\right)_{ij\ell} \tag{14}$$

$\eta_{ij\ell}$ = number of parcels within cell (i,j,ℓ)

The volume of the cell, $V_{ij\ell}$, is a known quantity. Consequently, an average intensive quality variable, usually a concentration or temperature, can be computed for each constituent in each cell by:

$$\Gamma_{ij\ell}^{k,*} = \frac{Z^k \zeta_{ij\ell}^{k,*}}{V_{ij\ell}} \tag{15}$$

where Z^k = an appropriate conversion factor to convert Γ^k to the units desired by the user (e.g., the factor for converting from cal/cm^3 to °F).

To complete the numerical scheme the contributions of the source/sink term must now be accounted for. The method used to model these contributions varies depending upon the type of mechanisms represented by ϕ^k. If the source/sink mechanism is simply a discharge of material into the system or a removal of material from it, parcels are either added to or removed from appropriate areas of the solution maxtrix.

Many source/sink mechanisms are of a more complicated type that describe interactions between the various constituents that may be present and between the constituents and the environment. These types of interactions may be specified by reaction rate or heat exchange expressions, or by equilibrium constraints. A reaction-rate type of mechanism, r^k, is a set of predefined functions that describe the rate of change of Γ^k as a function of all the species present in the system.

The change of Γ^k in cell (i,j,ℓ) during a given time step can be calculated explicitly by:

$$\Gamma_{ij\ell}^{k,n+1} = \Gamma_{ij\ell}^{k,*} + r^k\left(\Gamma_{ij\ell}^{m,*}\right)\Delta t \qquad m = 1,2,3...K \tag{16}$$

which can be evaluated directly or implicitly by

$$\Gamma_{ij\ell}^{k,n+1} = \Gamma_{ij\ell}^{k,*} + r^k\left(\Gamma_{ij\ell}^{m,n+1}\right)\Delta t \tag{17}$$

which can be solved using standard iterative matrix inversion methods.

If the source/sink mechanism is specified by constraining the system to be at equilibria at the end of each time step, the solution of a set of simultaneous nonlinear equations of the form shown in Equation 18 is required.

$$\Gamma_{ij\ell}^{k,n+1} = E_k\left(\Gamma_{ij\ell}^{m,*}\right) \qquad m = 1,2,3...K \tag{18}$$

where E_k represents a set of algebraic functions that specify the necessary conditions for equilibria to exist. These functions usually represent mass and charge balances and either mass-action expressions or relationships that specify the minimization of the Gibbs free energy. Systems of equations of this type are usually solved by a Newton-Raphson iteration or some other type of iterative procedure. The concentration values immediately following the advection-dispersion computations are used to provide starting values for the iterative procedure.

Once the concentration at the next time level, $\Gamma_{ij}^{k,n+1}$, has been determined the mass associated with each parcel is adjusted by the ratio of the change.

$$\left(\zeta_p^{k,n+1}\right)_{ij\ell} = \left(\frac{\Gamma_{ij\ell}^{k,n+1}}{\Gamma_{ij\ell}^{k,*}}\right)\left(\zeta_p^{k,*}\right)_{ij\ell} \tag{19}$$

The conversion of ζ to Γ does not necessarily have to be made prior to computing some types of source/sink term contributions, but Γ is usually a much more convenient quantity to work with than the extensive variable, ζ. For some simple rate expressions, such as an irreversible first order decay, the extensive variables can be modified directly:

$$\zeta_p^{k,n+1} = \zeta_p^{k,*} \; e^{-\lambda\Delta t} \tag{20}$$

where λ is the decay constant.

The solution can then proceed to the next time level.

Examples of Model Application

The Battelle Generalized Transport Model functions in three operational modes:

- Oil spill drift forecasting,
- Powerplant outfall analysis, and
- Groundwater contaminant plume prediction.

The operational modes differ primarily in the type of source/sink terms that have been coupled to them.

The model is currently in use in each operational mode by various governmental land state agencies. Samples of the output generated by each mode are shown in Figures 2-4. A document describing the details of the oil spill operational mode is available[3]. Documentation of the other two modes is currently under preparation.

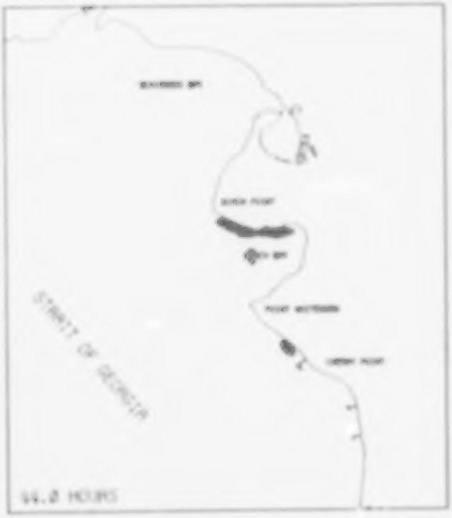

Figure 2. Oil Spill Operational Mode

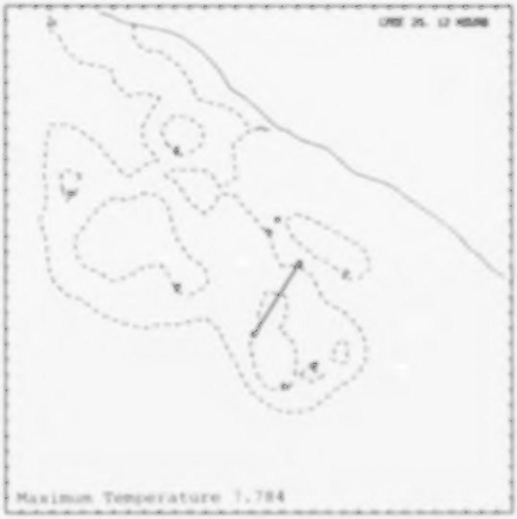

Figure 3. Powerplant Outfall Operational Mode

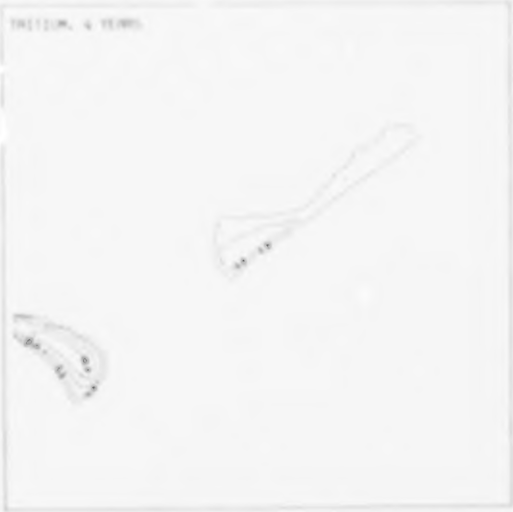

Figure 4. Groundwater Solute Operational Mode

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AN INTERACTIVE SYSTEM FOR TIME SERIES
ANALYSIS AND DISPLAY
OF
WATER QUALITY DATA

E. Buda
Michigan Department of Natural Resources
Lansing, Michigan
R. L. Phillips
C. N. Cederquist
J. E. Geister
Unidata, Incorporated, Ann Arbor, Michigan

SUMMARY

ADROIT is an interactive computer graphics system which is capable of rapid retrieval, statistical processing and graphical display of water quality data. It is used here to analyze trends in Soluble Ortho Phosphorus data collected on Michigan's Grand River, by the Michigan Department of Natural Resources between 1963 and 1974. Soluble Ortho Phosphorus concentrations are declining, and the decline is not due solely to increasing stream flows. Relationships between concentration, stream flow and loading rates for Soluble Ortho Phosphorus are examined. Further analysis, using ADROIT as an analytical tool, to define the impact of phosphorus abatement programs in Michigan is recommended.

ADROIT

ADROIT* (Automated Data Retrieval and Operations Involving Timeseries) is an interactive system which is capable of rapid retrieval, statistical processing and graphical display of water quality data. The system is basically an interpreter for a special-purpose problem-oriented programming language. It has been designed to produce retrospective statistical time series analyses of water quality data and, without further user intervention, to produce report-ready graphs of selected results. ADROIT comprises two major subsystems, the computational subsystem and the display subsystem. In addition, the system includes a stand-alone program called COMPOSE which is capable of additional graphical operations.

At the heart of the ADROIT Computational Subsystem (ACS) is a special purpose interpretive programming language. The language has been designed to properly handle timeseries data types, specifically those pertaining to water quality observations. Being an interpretive language, like BASIC, the computational task specified by the user is carried out immediately; there is no compilation step as in FORTRAN. The familiar data types of logical, string and numeric are present in ACS as well as novel data types such as obs and timeint. Each variable of type obs is actually a four-tuple of values, comprising the mean, sample variance, sample weight, and time of observation associated with water quality data. The introduction of this data type insures rigorous and proper handling of data observations in all arithmetic and statistical operations. The timeint data type has been introduced to permit arbitrary time period restriction and aggregation of data. Using variables of this type in conjunction with those of type obs enables the user to perform a wide range of water quality analyses.

In order to facilitate operations with timeseries data types, ADROIT provides a complete range of special built-in functions, as well as the standard numeric data type functions found in most programming languages. There are functions for extracting the components of an obs, for restricting data to a specified time interval, and for aggregating observations by specific intervals. In addition, there are statistical functions that compute the inverse normal, chi-squared, Fisher's F and Student's t distributions. These provide the building blocks for arbitrary complex statistical analyses that can be developed by the user.

A unique feature of ADROIT is the capability of building up a library of user-defined procedures. Thus, when the user finds there are functions that he frequently performs and finds useful, he can catalog them in a special procedure file by giving them a unique name. When the function is to be invoked, the user simply types its name (and any appropriate arguments) and the ACS executes the function immediately. For example, a procedure that computes both a water quality index and phosphate loading at a selected station is invoked by

```
WQIPHOS.('700026'.P665.TIME 70 THRU 74)
```

where the arguments are the station number, EPA parameter number, and the time interval for which the computations are to be performed.

The ADROIT Display Subsystem (ADS) is so flexible and provides such a wide range of capabilities that a user can, on the one hand, specify every aspect of the graph to be displayed or allow the system to produce all of its features automatically.

Just as the special data types in ACS are essential to the operation of the computational subsystem, a rigorous, canonical definition of a graph and its elements is a fundamental aspect of ADS. This graph description is maintained by the system in a form called a structure which the user can interact with to modify all or part of a graph. The structure is an ordered list of graph elements each of which requires one or more parameters to describe it. Typical graph elements would be the axes, tick marks, grid lines, labels, titles, etc. Independent x and y parameter (horizontal and vertical) specifications of each of these elements is under control of the user. Thus, he may elect to produce y-grid lines only and omit those for the x-axis. Among the display options available to the user are

.choice of linear or logarithmic axes
.point, line, or bar graph plotting of data
.curve smoothing or least squares data fitting
.absolute, relative or cumulative histograms
.general textual annotation
.three color Calcomp plots

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* ADROIT, A System for Water Quality Data Analysis and Display, Unidata, Incorporated, P. O. Box 2227, Ann Arbor, MI., June 1975.

Figures 1 through 15 are examples of finished graphs produced by ADROIT, using the facilities of both the computational and display subsystems.

Through ADROIT, large amounts of data extracted from the U.S. Environmental Protection Agency STORET system are available for rapid access and manipulation. Thus, the system is expected to be a valuable tool for research on the effectiveness of water quality control procedures.

Statistical Procedures Applied to Grand River Data

A number of ADROIT Procedures were used to process stream flow and soluble ortho phosphorus data for the Grand River at Grand Haven, Michigan.

The phosphorus data (mg/l) collected between 1963 through 1974 is plotted in Figure 1. During this period most of the data was collected monthly. Occasionally 2 samples per month were collected. There are numerous occasions when samples were not collected, particularly during winter months.

Figure 2 depicts this phosphorus data (mg/l) aggregated by year. The mean of the observations made during each year is plotted. An interval of ±1 standard deviation is also plotted with each mean.

The ADROIT Procedure INDICES. was used to compute the monthly seasonal indices.[1] These twelve indices (Table 1) indicate the fraction of each year's average phosphorus level (mg/l) that occured in each month, respectively. For January, 1.43 indicates that all January phosphorus levels (mg/l) averaged 43% higher than corresponding yearly averages over the 11 year period. If there were no seasonal influence, each month's level would be the same as every other month and the seasonal indices would all be close to 1.0. The seasonal indices for the phosphorus data (mg/l) are shown in Table 1.

The ADROIT Procedure DESEASON. was used to deseasonalize the phosphorus data (mg/l) by dividing each observation by the appropriate monthly index.[2] The deseasonalized phosphorus data (mg/l) is shown in Figure 3. The principle effect of this process is to reduce the variability of the original data by removing that portion of the total variability due to non-random seasonal effects. Figure 4 shows that the standard deviations have been reduced, while the annual sample means have remained the same as Figure 2. (NOTE: the standard deviations for 1973 and 1974 increased after deseasonalization due to partial yearly data.)

Figure 5 is a plot of the sample means of the phosphorus data (mg/l) with associated 90% confidence intervals. In this case the sample means and sample variances are used to estimate the interval within which the true population mean is likely to be 90% of the time. We are therefore inferring the value of the population means by using the sample statistics.

Three ADROIT Procedures were used to compute Figure 5. Figure 5 is the best estimate of the mean phosphorus concentration for each year, with seasonal and serial correlation effects accounted for. Procedure SERIAL. was used to compute the 1st order serial correlation coefficient, R, for the deseasonzlized phosphorus data.[3] For this period of record, R = 0.43. To determine if this value of R was significant for the number of observations used, the 1st order serial correlation coefficient and 95% confidence limits were computed for an artificial, normal, random time series.[4] This was done with Procedure TESTP. Since R = 0.43 for our data is greater than the upper confidence limit of the random time series of 0.16, R is significant at the 95% level.

Procedure VARADJ. is used to adjust the variances of the deseasonalized phosphorus data to account for the serial correlation.[5] In effect the variances were increased by 15-53% depending on the number of observations each year. These adjustment factors were computed on the basis of an artificial time series (first order Markov process) with the same degree of serial correlation. Applying these factors to our data is an approximation, but it allows us to adjust for serial correlation and arrive at a better estimate of the confidence intervals. As the sample size decreases, the factors increase.

In a similar manner, the flow data is processed and the results are shown in Table 2 and Figures 6 through 10.

Figures 11 and 12 (previously presented as Figures 5 and 10) are plots of the mean soluble phosphorus concentration (mg/l) and stream flow (cfs) respectively, with 90% confidence intervals. All data has been deseasonalized. Since stream flow affects concentration data, the phosphorus loading rate has been computed as a way to consider changes in concentration and flow together.

Procedure LOAD. was used to compute these loadings. The instantaneous loading rate is the product of the concentration and stream flow at that time. (In addition to a unit constant) Because there are occasions when more than one concentration sample or flow measurement per month were made, procedure LOAD. aggregates by month first, to assign a single flow and concentration observation for each month. Then for those months with corresponding concentration and flow observations the product is taken to yield a monthly loading observation.

Procedure LOAD. operated on deseasonalized concentration and flow data and therefore the loading data is deseasonalized. Procedures SERIAL. and TESTP. were used to yield a serial correlation coefficient of 0.30 which is significant at the 95% level when compared to the highest expected value of 0.18.

Procedure VARADJ. was used to adjust the variances for this serial correlation and Figure 13 is a plot of the sample means of the phosphorus loading (lbs/day) rate with associated 90% confidence intervals.

Figure 14 is a plot of stream flow versus soluble phosphorus concentration (mg/l) for the period 1963 through 1974. It was produced using procedure VERSUS. which aggregates all data by month, and assigns plotting pairs for each month. The regression line is also plotted. Procedure LINCOR. was used to compute the linear correlation coefficient which was - 0.297.

Similarly, Figure 15 is a plot of stream flow versus soluble phosphorus loading (lbs/day) for the same data. The linear correlation coefficient is +0.788.

Discussion of Results

Soluble Phosphorus Concentrations Over Time

A major objective of this analysis is to determine if water quality is improving or not. Soluble ortho phosphorus, an important nutrient for aquatic organisms, is examined with these statistical techniques as one of a number of parameters which can be analyzed similarly. Water Quality is improving if the phosphorus concentration is decreasing over time in a statistically significant way.

SOLUBLE ORTHO PHOSPHORUS AS P, MG/L

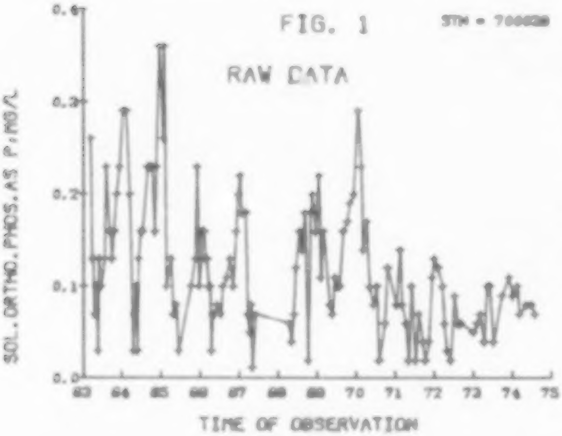
FIG. 1

RAW DATA

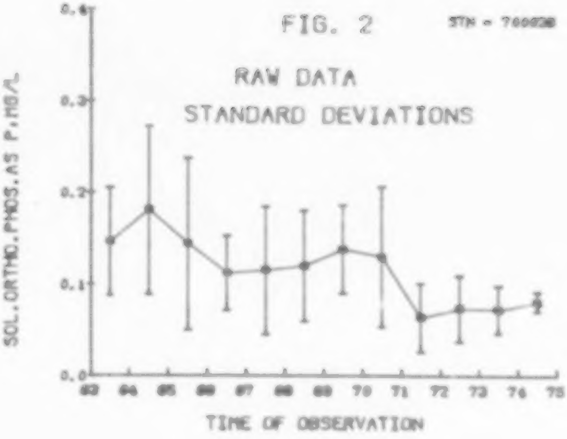
FIG. 2

RAW DATA
STANDARD DEVIATIONS

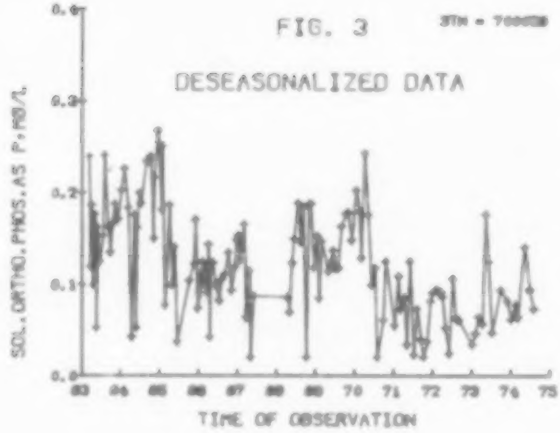
FIG. 3

DESEASONALIZED DATA

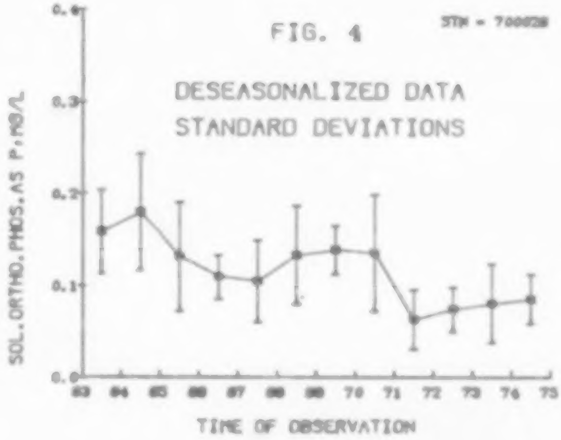
FIG. 4

DESEASONALIZED DATA
STANDARD DEVIATIONS

TABLE 1

SOLUBLE ORTHO PHOSPHORUS SEASONAL INDICES

JAN	1.43	JUL	0.85
FEB	1.28	AUG	0.95
MAR	1.09	SEP	0.98
APR	0.70	OCT	0.96
MAY	0.57	NOV	1.06
JUN	0.80	DEC	1.34

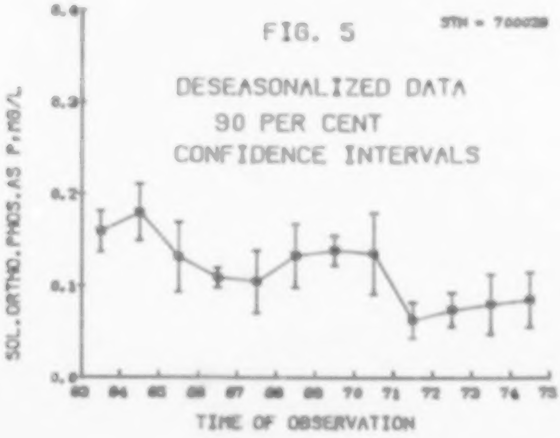
FIG. 5

DESEASONALIZED DATA
90 PER CENT
CONFIDENCE INTERVALS

STREAM FLOW, CUBIC FT/SEC

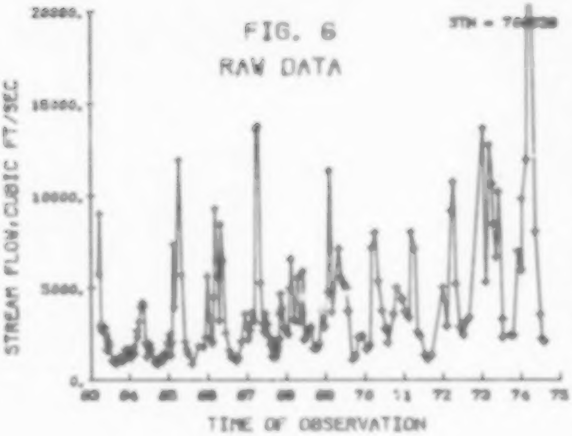
FIG. 6
RAW DATA

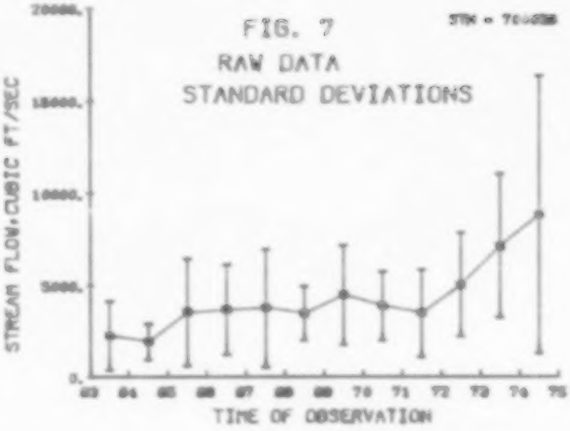
FIG. 7
RAW DATA
STANDARD DEVIATIONS

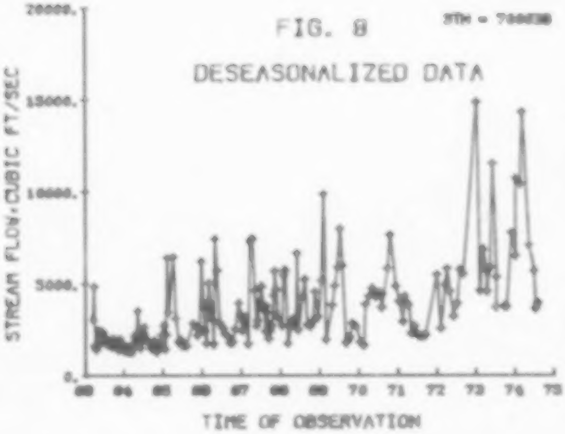
FIG. 8
DESEASONALIZED DATA

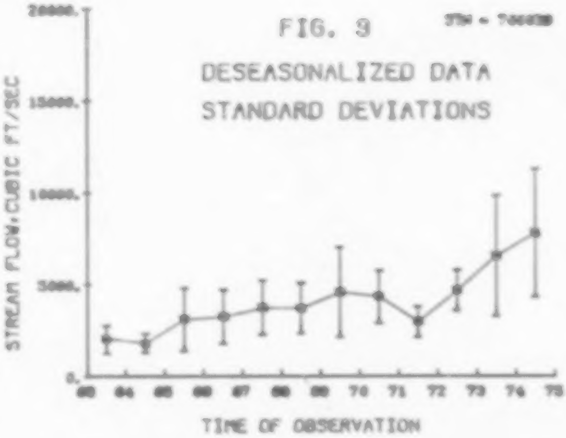
FIG. 9
DESEASONALIZED DATA
STANDARD DEVIATIONS

TABLE 2

STREAM FLOW
SEASONAL INDICES

JAN	0.92	JUL	0.63
FEB	1.15	AUG	0.55
MAR	1.86	SEP	0.62
APR	1.85	OCT	0.66
MAY	1.14	NOV	0.83
JUN	0.89	DEC	0.91

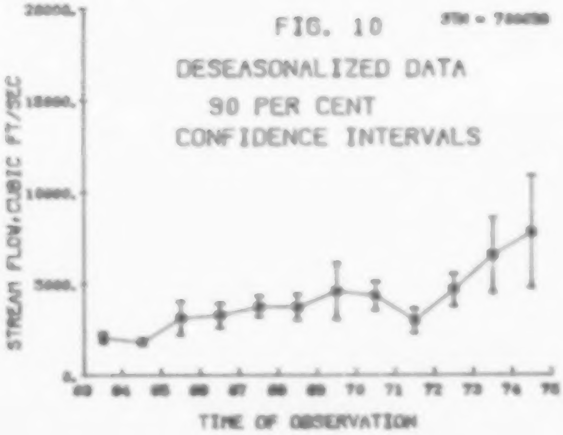
FIG. 10
DESEASONALIZED DATA
90 PER CENT
CONFIDENCE INTERVALS

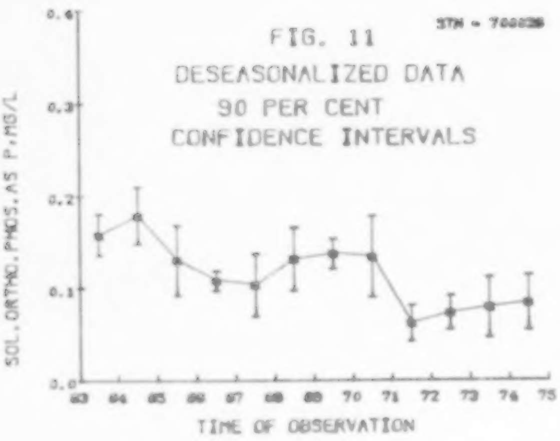

FIG. 11

DESEASONALIZED DATA
90 PER CENT
CONFIDENCE INTERVALS

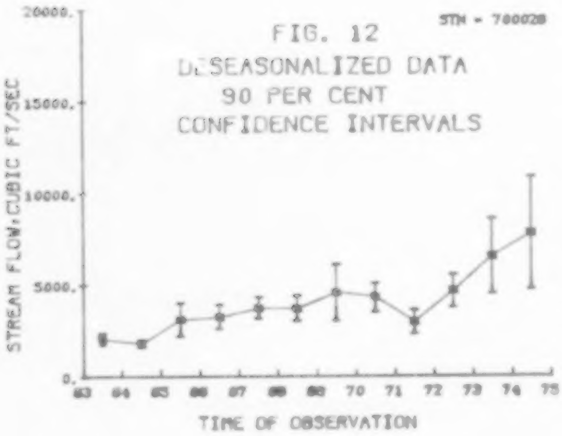

FIG. 12

DESEASONALIZED DATA
90 PER CENT
CONFIDENCE INTERVALS

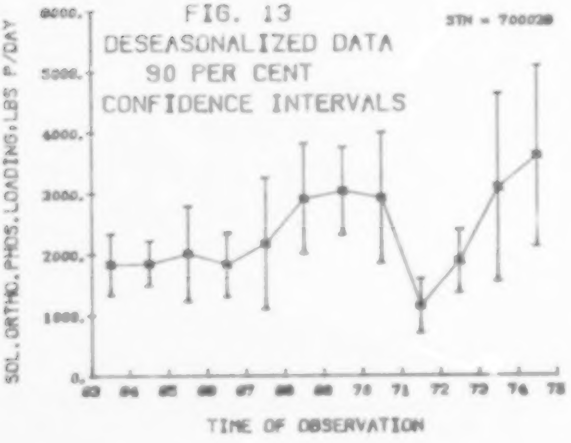

FIG. 13

DESEASONALIZED DATA
90 PER CENT
CONFIDENCE INTERVALS

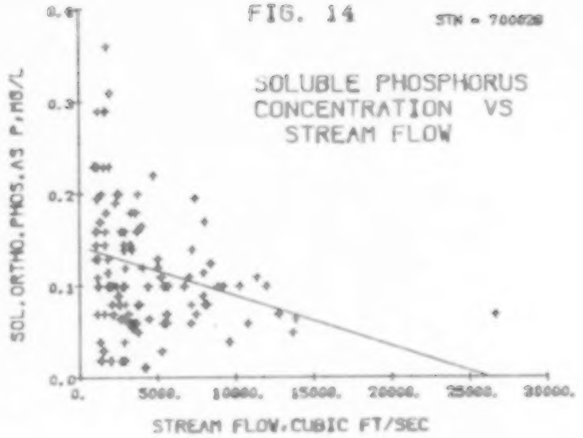

FIG. 14

SOLUBLE PHOSPHORUS
CONCENTRATION VS
STREAM FLOW

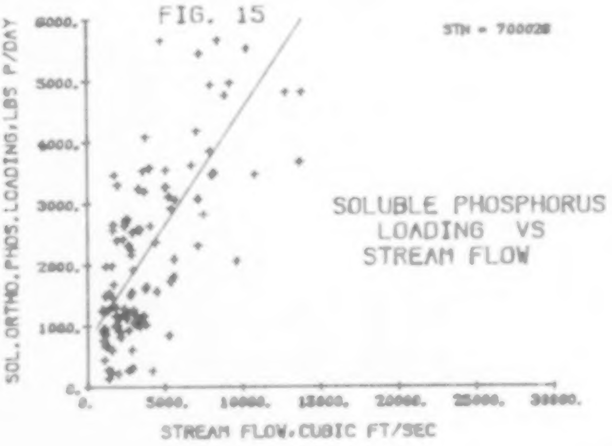

FIG. 15

SOLUBLE PHOSPHORUS
LOADING VS
STREAM FLOW

Figure 9 indicates that the phosphorus concentration has declined. The confidence intervals for any two years may be compared. If there is no overlap of the intervals (i.e. 1963 compared to 1972) the difference in the means may be considered significant.* We conclude therefore that the phosphorus concentrations in the early 1970's are significantly lower than levels in the early 1960's. Indeed the data could be aggregated over 5 year periods to demonstrate this. The confidence intervals were computed using the t distribution, well suited for small samples (less than 30 observations), the data was deseasonalized to remove an important non-random component of the sample variance and the variance was adjusted to account for the serial correlation of the data. This analysis sequence can be applied to other parameters to produce interval estimates of the population mean.

Stream Flow Levels Over Time

We now must consider some possible cause and effect relationships. It must be emphasized that this data base of monthly observations may not be sufficient to answer all questions we will now raise. However, these statistical techniques will give us some insight.

Figure 10 is the stream flow analogy of Figure 9. It indicates that stream flow has increased significantly, since 1963. The large confidence intervals for 1973 and 1974 are due in part to reduced sample size.

Concentration - Stream Flow Relationships

Is concentration decreasing because flow is increasing? This question is addressed in Figures 11 and 12. Between 1963 and 1971 concentration declines while flow increases. However from 1972 through 1974 concentration remains at about the same level (the overlap of the confidence intervals implies the apparent increase is not significant) while flow continues to increase. This latter period seems to contradict the original relationship. The relationship is unclear.

Figure 13 is the phosphorus loading rate resulting from the concentration and flow data of Figures 11 and 12. The loading rate appears to be influenced most by the stream flow, with concentration acting as a relative constant in the loading product. The best way to discern the relationships between concentration, flow and loading is shown in Figures 14 and 15.

Figure 14 plots concentration versus associated streamflow. The relationship is poor, as demonstrated by a wide range of concentration observations associated with flows of 5000 cfs and less. A regression line is shown. The linear correlation coefficient of 0.297 indicates a poor linear relationship. Figure 14 does not mean that concentration is not a function of flow, but rather, flow is not the only factor influencing soluble phosphorus concentration. It is likely that storm intensity and duration along with other hydrographic factors are significant. We must conclude however that the apparent decline of phosphorus concentrations of Figure 11 cannot be attributed to flow. Since phosphorus removal facilities for municipal treatment plants were constructed during this period, it is possible that Figure 11 reflects this change. Further analysis is necessary to define this relationship.

As expected, Figure 15 demonstrates that there is a strong relationship between streamflow and soluble phosphorus loading rates. The linear correlation coefficient is +0.785 indicating a good linear correlation. In light of **Figure** 14, we must conclude that soluble ortho phosphorus loading rates reflect the strong influence of flow in the loading rate product, and that loading rates as a parameter for measuring trend provide little new information in this case.

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[1] Spiegel, M.R., "Theory and Problems of Statistics", (Schaum's Outline Series, McGraw-Hill Book Co., 1961), p. 233.

[2] Spiegel, p. 299.

[3] Yevdjevich, M.V., "Statistical and Probability Analysis of Hydrologic Data", (Handbook of Applied Hydrology, McGraw-Hill Book Co., 1964), p. 8-79.

[4] Yevdjevich, p. 8-82.

[5] Yevdjevich, p. 8-86.

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* The t test may be applied as a rigorous test, but this graphical method is a good approximation.

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